# DEPARTMENT OF ENERGY FY 1997 CONGRESSIONAL BUDGET REQUEST ENERGY SUPPLY, RESEARCH AND DEVELOPMENT (Tabular dollars in thousands, Narrative in whole dollars)

#### **BASIC ENERGY SCIENCES**

#### **PROGRAM MISSION**

The mission of the Basic Energy Sciences (BES) program is to expand scientific knowledge needed to develop new energy technologies, to improve existing energy technologies, and to aid economic growth.

The GOAL of the BES program is to:

Support the highest quality research through thorough and fair peer review; operate major scientific user facilities, such as synchrotron radiation and neutron sources, for broad support of many forefront research areas; plan, design, and construct advanced facilities to meet future research needs. To accomplish the mission, BES supports basic scientific research at universities, national laboratories and industrial research laboratories (primarily through the Small Business Innovation Research program) in materials sciences, chemical sciences, engineering, geosciences, and energy biosciences.

#### The OBJECTIVES related to these goals are:

- 1. To CONTRIBUTE TO SUSTAINABLE ENERGY PRODUCTION AND USE Conduct basic research that creates scientific and engineering knowledge in support of Department of Energy mission thrusts to accelerate the utilization and development of energy technologies in a safe and environmentally compatible manner.
- 2. To PROVIDE WORLD CLASS SCIENTIFIC FACILITIES Provide and operate major user facilities needed for DOE research and foster research partnerships with industry and the entire scientific community. These scientific facilities include synchrotron radiation sources, neutron sources, and electron beam microanalytical instruments which are essential forefront research tools that scientists use to advance knowledge and develop new products, materials, and manufacturing processes.

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

3. To ENSURE THAT RESEARCH RESULTS ARE WIDELY KNOWN, VALUED AND USED - Promote open communications and the transfer of information, know-how and technology among university, government, and the private sector. Activities include peer review of all research activities and strong coordination and planning with the energy technology offices of the Department, collocation of researchers, input from all stakeholders, and in-depth workshops and conferences between scientists, engineers, and technologists with management sponsorship and participation. The national laboratories and universities are excellent resources to bring about these important interactions.

#### Scientific Facilities Utilization:

The Basic Energy Sciences program request includes \$277,636,000 to maintain support of the Department's scientific user facilities. Approximately 20% of this amount is associated with the continuation of the science user facilities initiative contained in the FY 1996 budget request. This investment will provide research time for thousands of scientists in universities, Federal agencies, and U.S. companies. It will also leverage both Federally and privately sponsored research, consistent with the Administration's strategy for enhancing the U.S. National science investment. The proposed funding supports the number of users served in FY 1996, which was an increase of several thousand over FY 1995 levels, and will maintain the quality of service and availability of facility resources to users, including university and government scientists, as well as private companies who rely on unique facilities for their basic research needs. The proposed funding level will also provide for efficient utilization of high technology facilities, which are generally oversubscribed by factors of two to three. Research communities that will benefit from this initiative include structural biology, materials sciences, superconductor technology, and medical research and technology development.

#### PERFORMANCE MEASURES:

The Department has developed performance measures for the results of its basic research activities. General performance measures of program outputs for basic research include such metrics as the number of scientists supported, the number of students earning advanced degrees, the number of scientific publications in peer-reviewed journals, the number of awards from professional organizations, and the number of citations in scientific publications. Metrics for the transfer of new knowledge to a technology application include the number of cooperative agreements with industry, the number of projects resulting in support from a DOE Energy Technology program, the number of invention records and patents, and the number of industry users at the major scientific user facilities. For construction projects, metrics can include costs and schedule milestones completed against approved project baselines. These performance measures are easily tabulated, commonly used, and begin to provide a framework for evaluating program efficiency. However, the most descriptive indicators in this area are qualitative rather than quantitative measures. In order to measure outcomes, or program effectiveness, the impact of the research outputs must be assessed in terms of the quality of the new knowledge gained, its usefulness to technology development, and its longer-term benefit to society. Although there are limited and expensive methods for evaluating the quality of science through peer-review metrics, no metric exists that can accurately measure

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

science's impact on technology and society. The extent of industrial interest is a measure of the value of the research. BES has been involved in over 500 collaborations with industry. These collaborations extend over all sectors of the economy.

#### SIGNIFICANT ACCOMPLISHMENTS AND PROGRAM SHIFTS:

- The existing National User Facilities will operate more effectively (in some cases with substantial increases in operating hours, and in others, with the implementation of modern state-of-the-art instrumentation which will use the neutron and photon beams more effectively) with more experiments and more users as a consequence of the President's User Facility Initiative in FY 1996. This initiative will be sustained in FY 1997 with \$277,636,000 included to maintain support of the Department's Scientific User Facilities.
- O Commissioning of the Advanced Photon Source Storage Ring began in FY 1995 and a circulating current of 8.5 milliamperes was achieved resulting in the first x-ray beams at this third generation x-ray source. The design of 100 milliamperes was reached in January of 1996.
- o Preconstruction research and development, environmental impact statement, and conceptual design will be performed for a Spallation Neutron Source. In addition, options will be evaluated for upgrading existing reactor and spallation sources as near-term solutions for providing neutrons while the next generation Spallation Neutron Source is being developed.
- o Construction of the Combustion Research Facility, Phase II will continue in FY 1996 and FY 1997 with completion scheduled for FY 1999.
- The program assumes responsibility for the management of the Experimental Program to Stimulate Research (EPSCoR) in FY 1996.

#### BASIC ENERGY SCIENCES

(Dollars in thousands)

#### PROGRAM FUNDING PROFILE

	FY 1995 Comparable Appropriation	FY 1996 Original Appropriation	FY 1996 Real & Comp Adjustments	FY 1996 Comparable Adjusted	FY 1997 Budget Request
Research	٠	•		·	
Materials Sciences	\$263,598	\$367,400	-\$30,295	a/ \$337,105	\$334,560
Chemical Sciences	154,446	198,400	-21,357	b/ 177,043	173,370
Engineering and Geosciences	34,635	41,700	-2,889	c/ 38,811	41,250
Energy Biosciences	26,935	30,200	-1,500	d/ 28,700	28,185
Advanced Energy Projects	. 0	12,300	-12,300	e <i>l</i> 0	0
Applied Mathematical Sciences		116,500	-116,500	f/ 0	0
Program Direction	0	9,500	<b>-9,500</b>	g/ 0	0
Related Capital Funding	58,734	. 0	62,931	62,931	64,810
Subtotal, Research	538,348	776,000	-131,410	644,590	642,175
Construction	58,379	15,661	-5,675	h/ 9,986	11,500
Subtotal, Basic Energy Sciences	596,727	791,661	-137,085	654,576	653,675
Adjustment	j/	k/	3,783	m/j/	0
Total, Basic Energy Sciences	\$589,255 n/	\$774,493	-\$133,302	\$641,191	\$653,675

a/ Reprogramming to the Indian Energy Resources programs (\$-1,135,000); redistribution between subprograms within Basic Energy Sciences (\$+3,415,000); and comparability transfer to Related Capital Funding (\$-32,575,000).

b/ Reprogramming to the Indian Energy Resources programs (\$-593,000); redistribution between subprograms within Basic Energy Sciences (\$+1,500,000); and comparability transfer to Related Capital Funding (\$-22,264,000).

c/ Reprogramming to the Indian Energy Resources programs (\$-124,000); redistribution between subprograms within Basic Energy Sciences (\$-1,011,000); and comparability transfer to Related Capital Funding (\$-1,754,000).

d/ Reprogramming to the Indian Energy Resources programs (\$-87,000); redistribution between subprograms within Basic Energy Sciences (\$-750,000); and comparability transfer to Related Capital Funding (\$-663,000).

e/ Reprogramming to the Indian Energy Resources programs (\$-65,000); redistribution between subprograms within Basic Energy Sciences (\$-292,000); and comparability transfer to Computational and Technology Research (\$-11,943,000).

- f/ Reprogramming to the Indian Energy Resources programs (\$-482,000); redistribution between subprograms within Basic Energy Sciences (\$-2,862,000); and comparability transfer to Computational and Technology Research (\$-113,156,000).
- g/ Comparability transfer to Energy Research Energy Supply Research and Development Program Direction (\$-9,500,000).
- h/ Redistribution of AIP over \$2,000,000 to Related Capital Funding for AIP under \$2,000,000 (\$-5,675,000).
- j/ Share of Energy Supply Research and Development general reduction for use of prior year balances assigned to this program on a comparable basis. The total general reduction is applied at the appropriation level.
- k/ Share of Energy Supply Research and Development general reduction for use of prior year balances assigned to this program on a non-comparable basis. The total general reduction is applied at the appropriation level.
- m/ Comparability transfer to Computational and Technology Research.
- n/ Excludes \$9,859,000 which has been transferred to the SBIR program and \$493,000 which has been transferred to the STTR program.

#### Public Law Authorizations:

Public Law 95-91 "Department of Energy Organization Act" (1977)

## BASIC ENERGY SCIENCES (Dollars in thousands)

#### PROGRAM FUNDING BY SITE

Field Offices/Sites	FY 1995 Comparable Appropriation	FY 1996 Original Appropriation	FY 1996 Real & Comp Adjustments	FY 1996 Comparable Appropriation	FY 1997 Budget Request
Albuquerque Operations Office					
Los Alamos National Laboratory	\$11,655	\$32,187	-\$12,907	\$19,280	\$17,272
Sandia National Laboratories	20,023	25,630	-4,725	20,905	28,021
Chicago Operations Office					
Ames Laboratory	15,475	21,349	-5,321	16,028	16,227
Argonne National Laboratory	177,375	155,725	-10,214	145,511	141,579
Brookhaven National Laboratory	71,949	83,115	-863	82,252	80,467
Fermi National Accelerator Laboratory	0				
Golden Field Office					
National Renewable Energy Laboratory	3,533	5,387	-1,150	4,237	3,790
Idaho Operations Office					
Idaho National Engineering Laboratory	3,660	3,119	-95	3,024	3,138
Oakland Operations Office					
Lawrence Berkeley National Laboratory	54,398	90,687	-27,821	62,866	62,011
Lawrence Livermore National Laboratory	5,709	20,452	-14,794	5,658	4,910
Stanford Linear Accelerator Center	16,095	21,459	0	21,459	20,996
Oak Ridge Operations Office					
Oak Ridge Institute for Science & Education	455	725	0	<b>725</b>	424
Oak Ridge National Laboratory	83,590	96,739	-11,395	85,344	90,502
Continuous Electron Beam					
Accelerator Facility	0	150	-150	0	0
Richland Operations Office					
Pacific Northwest National Laboratory	. 11,759	11,655	-523	11,132	11,264
All Other Sites a/	121,051	223,282	-47,127	176,155	173,074
Subtotal	596,727	791,661	-137,085	654,576	653,675
Adjustment	-7,472 b/	b/	3,783 c/	d/	0
TOTAL	\$589,255	\$774,493	-\$133,302	\$641,191	\$653,675

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



b/ Share of Energy Supply Research and Development general reduction for use of prior year balances assigned to this program on a non-comparable basis.

c/ Share of Energy Supply Research and Development general reduction for use of prior year balances assigned to this program on a comparable basis.

c/ Comparability transfer to Computational and Technology Research.

## BASIC ENERGY SCIENCES PROGRAM OBJECT CLASS SUMMARY (Dollars in thousands)

	•	FY 1995		FY 1996			
		Comparable	Non-Comp	Comparable	Non-Comp	FY 1997	
	Direct Funding:						
	Personnel compensation:				•		
11.1	Full-time permanent		\$5,090		\$6,061		
11.3	Other than full-time permanent		42		60		
11.5	Other personnel compensation		231		328		
11.8	Special personal services payments		0_		0_		
11.9	Total personnel compensation	. 0	5,363	0	6,449	0	
12.1	Civilian personnel benefits		979		1,324		
13.0	Benefits for former personnel		157	•	200		
21.0	Travel and transportation of persons		328		356		
22.0	Transportation of things				•		
23.1	Rental payments to GSA						
23.2	Rental payments to others						
23.3	Communications, utilities, and miscellaneous charges				•		
24.0	Printing and reproduction						
25.1	Advisory and assistance services	75	2,016		1,995	. 0	
25.2	Other services	6,187	9,717	50,298	64,828	53,868	
25.3	Purchases of goods and services		-				
	from Government accounts						
25.4	Operation and maintenance of facilities	364,505	455,877	410,335	493,344	408,497	
25.5	Research and development contracts	Ť					
25.7	Operation and maintenance of equipment						
26.0	Supplies and materials				•		
31.0	Equipment	38,854	37,749	48.339	56,043	45,695	
32.0	Land and structures	74,782	66,468	23,901	23,901	30,615	
41.0	Grants, subsidies and contributions	105,454	124,910	109,500	128,500	115,000	
99.0	Subtotal, obligations	589,857	703,564	642,373	776,940	653,675	
	Reimbursable Obligations	Ó	0	0	O	•	
99.9	Total Obligations	589,857	703,564	642,373	776,940	653,675	
	Recovery of prior year obligations	-36	-58	-17	-26		
	Unobligated balance avail, start of year	-1,672	-1,081	-1,165	-2,421		
	Unobligated balance avail, end of year	1,106	2,421	0	0		
	Budget Authority	\$589,255	\$704,846	\$641,191	\$774,493	\$653,675	

#### **BASIC ENERGY SCIENCES**

## MATERIALS SCIENCES (Tabular dollars in thousands, Narrative in whole dollars)

#### I. Mission Supporting Goals and Objectives:

The Materials Sciences subprogram supports energy related fundamental scientific research in materials and the operation of national scientific user facilities that support the energy mission needs and Strategic Plan of the Department. The facility operations activities funded in this subprogram are described in a separate "Major User Facility" section of this budget. Facilities supported include the National Synchrotron Light Source (NSLS), the High Flux Beam Reactor (HFBR), the Intense Pulsed Neutron Source (IPNS), the Stanford Synchrotron Radiation Laboratory (SSRL), the Manuel Lujan, Jr. Neutron Scattering Center (MLJNSC), the Advanced Light Source (ALS), and the Advanced Photon Source (APS).

Materials Science is an enabling technology. The efficiency, economics, environmental acceptability, and safety of all energy generation, conversion, transmission, and conservation technologies are limited by the performance of materials. Research in Materials Sciences is concerned with the discovery and optimization of the behavior and performance of materials in these energy technologies. This research seeks to understand the synergistic relationship among the synthesis, processing, structure, properties, behavior, and performance of materials in such energy technologies.

#### II. Funding Schedule:

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
Materials Sciences Research	\$129,773	\$162,669	\$161,480	<b>\$-</b> 1,189	- 0.7%
Facilities Operations	133,825	<u>174,436</u>	<u>173,080</u>	<u>- 1.356</u>	<u>- 0.8%</u>
Total, Materials Sciences	<u>\$263,598</u>	<u>\$337,105</u>	<b>\$334,560</b>	<b>\$-2.545</b>	- 0.8%

#### Performance Summary: MATERIALS SCIENCES (Cont'd)

#### FY 1995 Accomplishments:

III.

- O Synthesis and processing research on advanced materials such as the design of advanced chemical vapor deposition reactors for the fabrication of semiconductors has led to materials with enhanced behavior and performance and reductions in the waste, pollution, and cost associated with the production of new and modified materials.
- o Improved scientific understanding of corrosion mechanisms, achieved partly through experimental techniques such as optically pumped nuclear magnetic resonance of surfaces, x-ray characterization of corroding surfaces, and direct atom imaging and verification of surface diffusion could lead to economic savings as well as improved performance in energy technologies. Aqueous, galvanic, and gaseous corrosion damage costs the U.S. economy 5% of the Gross Domestic Product per year.
- o Fundamental research on energy losses in high-performance magnets will lead to improved efficiency motors and transformers. Magnetic energy losses in motors and transformers cost the U.S. economy \$16 million per year.
- O A basic understanding of the welding and joining of metals and ceramics has led to improved welding procedures for dissimilar metals and for the joining of metals to ceramics. Significantly improved welds reduce catastrophic failures and increase lifetime of components in energy power plants.
- Improved understanding of the high-rate and superplastic forming of metals and alloys has been gained through fundamental theory and computer simulation of the process. Better understanding of interfacial deformation mechanisms during high-rate metal forming led to the successful fabrication of lightweight alloys for components, such as a door panel produced by a domestic automobile manufacturer.
- o Improved understanding of neutron-induced irradiation damage has led to more accurate predictive modelling and failure prevention in on-line commercial nuclear power plants.
- o New analytic methods involving synchrotron irradiation have led to more sensitive analyses for catalysts and trace impurities in surfaces and interfaces.

#### Performance Summary: MATERIALS SCIENCES (Cont'd)

III.

- o Neutron scattering experiments have provided an understanding of magnetic structure and excitations, hydrocarbons, residual stress mapping and atomic arrangements in a broad range of materials (polymer blends, metals, alloys, and ceramics).
- o Basic research on the properties and behavior of high-temperature load bearing, structural ceramics, and ceramic matrix composites has made these advanced materials move closer towards acceptance in large-scale applications for high-speed cutting tools and fuel efficient and low pollutant engines and turbines.
- o Basic research on sound wave scattering by microscopic flaws in solid materials has led to improved nondestructive diagnostics and early warning of impending failure.
- o Understanding of the effects of defects produced by processing of ceramics and polymers has led to significantly improved performance for ceramic and polymer electrolytes for batteries and fuel cells.
- o Understanding the grain boundary structure and microchemistry, phase equilibria, processing and behavior of ordered intermetallic alloys has led to increased commercial application for heat, load, wear and corrosion resistant applications.
- o Basic research on the interaction of charged particle beams with solid surfaces has led to the commercialization of surface modification and ion beam implantion technologies for improved corrosion, wear resistance, and surface load bearing applications.
- o New understanding in the processing of high-temperature superconductors with improved current-carrying capability has brought them closer to eventual commercialization.
- Coordinated multi-institutional and multidisciplinary basic research projects were initiated in response to workshops under the Center of Excellence for Synthesis and Processing of Advanced Materials concerning conventional and superplastic metal forming, materials joining, nanostructured materials for energy applications, microstructural engineering with polymers, tailored microstructures in hard magnets, processing for surface hardness, and mechanically reliable surface oxides for high temperature corrosion resistance. The Center of Excellence for Synthesis and Processing is coordinated by Sandia National Laboratories and involves work at 13 national laboratories.
- o Funding in the amount of \$5,433,000 and \$272,000 has been transferred to the SBIR and STTR programs, respectively.

#### FY 1996 Planned Accomplishments (to date and planned):

- o Basic scientific investigations will be continued in all of the topics that correspond to the above FY 1995
  Accomplishments and in all of the seven projects initiated in FY 1995 under the Center of Excellence for the Synthesis and Processing of Advanced Materials.
- O Coordinated multi-institutional and multidisciplinary new projects that will be initiated in response to workshops under the Center of Excellence for the Synthesis and Processing of Advanced Materials concerning high efficiency photovoltaics and bulk metallic glasses.
- o Research will be initiated concerning photonic band gap materials that may lead to improved signal transmission and processing using light instead of electrons.
- o Research to study the role of defects in advanced permanent magnet materials with a goal of enhancing the magnetic strength will be initiated that could lead to significant reductions in the energy losses and cost of operation of motors.
- o Initiate research using new techniques to study the nanometer-scale magnetic structure-property relationships in materials surfaces, thin films, and multilayers that will lead to an improved understanding of new phenomena such as "giant magnetoresistance" and "spin valve" effects which have the potential to enhance existing electronics technologies.
- o Peer-reviewed basic materials research will be initiated that fulfills the needs and opportunities that were identified in the joint Basic Energy Sciences-National Science Foundation Vehicles for the Future workshop that was held in January 1995.
- o Peer-reviewed basic materials research will be initiated that will be responsive to needs and opportunities relating to total product lifecycle and recyclability.
- o Peer-reviewed basic materials research will be initiated that will be responsive to needs and opportunities relating to the minimization, safe transport, and containment of waste and hazardous materials.
- o Preconstruction research and development, environmental impact statement, and Conceptual Design will be initiated for a Spallation Neutron Source. In addition, options will be evaluated for upgrading existing reactor and spallation sources as near-term solutions for providing neutrons while the next generation Spallation Neutron Source is being developed.

- o Experiments involving very high resolution, analytical, and high voltage environmental cell electron beam microcharacterization will be carried out at the Electron Microscopy Center for Materials Research, Center for Microanalysis of Materials, National Center for Electron Microscopy and Shared Research Equipment Program.
- o Funding in the amount of \$6,599,000 and \$494,000 has been budgeted for the SBIR and STTR programs, respectively.

#### FY 1997 Planned Accomplishments:

- o Basic scientific investigations will be continued in all of the topics that are planned for FY 1996 with slight reductions in the areas of Solid State Physics, Materials Chemistry, Metallurgy and Ceramics..
- o Initiate research concerning the surface and interface properties and behavior of quasicrystals for materials with improved corrosion resistance.
- o Initiate research concerning charge transport across superconductor-semiconductor and superconductor-metal interfaces to develop understanding on joining of superconductors with normal materials.
- o Initiate research concerning the kinetics of phase transformations in the heat affected zones of welds to improve understanding of failure in welds.
- o Initiate research concerning the synthesis of non-equilibrium materials using laser-molecular beam epitaxy to synthesize new materials with improved properties.
- o Peer-reviewed basic materials research that fulfills the needs and opportunities that were identified in the joint Basic Energy Sciences-National Science Foundation "Basic Research Needs for Environmentally Responsive Technologies of the Future" Workshop that was held in January 1996 will be continued.
- o Peer-reviewed basic materials research that is responsive to needs and opportunities relating to total product lifecycle will be continued.

#### Performance Summary: MATERIALS SCIENCES (Cont'd)

III.

- o Peer-reviewed basic materials research that is responsive to needs and opportunities relating to the minimization, safe transport, and containment of waste and hazardous materials will be continued.
- Conceptual Design, environmental impact statement, and preconstruction research and development for the Spallation Neutron Source will be continued. In addition, options will be evaluated for upgrading existing reactor and spallation sources as near-term solutions for providing neutrons while the next generation Spallation Neutron Source is being developed.
- o Funding in the amount of \$8,364,000 has been budgeted for the SBIR program.

#### Explanation of Funding Changes FY 1996 to FY 1997:

Reduced funding levels will cause slight decreases in research in the areas of solid state physics, materials chemistry, metallurgy, and ceramics will be decreased (\$-1,189,000).

Overall operating time at user facilities such as HFBR, IPNS, NSLS, SSRL, LANSCE, and ALS will be maintained at slightly below the FY 1996 level (\$-1,356,000). Operation of the Advanced Photon Source is initiated.

#### **BASIC ENERGY SCIENCES**

## CHEMICAL SCIENCES (Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives</u>:

The Chemical Sciences subprogram activity supports a broad range of basic research in molecular, atomic and chemical engineering sciences necessary for both improvements in existing energy technologies and that provides the necessary underlying science base that may lead toward the development of new energy technologies. The program is focussed upon the creation of new knowledge that will impact a broad spectrum of energy technologies. Major chemical sciences research efforts are important to the more efficient conversion of solar energy as well as improved catalytic processing to produce fuels, electricity or chemicals; more efficient and cleaner combustion; better utilization of the nation's carbon-containing resources including natural gas, oil, and coal; improved approaches to environmental concerns related to energy production; more sensitive and specific monitoring of physical and chemical processes; and the advancement of fusion and plasma related sciences.

In addition, the Chemical Sciences program provides support for major scientific user facilities which are operated for the benefit of the entire scientific community. The facility operations funded in this subprogram are described in a separate "Major User Facility" section in this budget. Facilities supported include: the National Synchrotron Light Source (NSLS), the High Flux Isotope Reactor (HFIR), the Radiochemical Engineering Development Center (REDC), the Stanford Synchrotron Radiation Laboratory (SSRL), and the Combustion Research Facility (CRF).

#### II. Funding Schedule:

Program Activity	<u>FY 1995</u>	FY 1996	FY 1997	\$ Change	% Change
Chemical Sciences Research	\$100,629	\$114,972	\$112,105	\$- 2,867	- 2.5%
Facilities Operations	<u>53,817</u>	<u>62,071</u>	61,265	<u>- 806</u>	<u>- 1.3%</u>
Total, Chemical Sciences	<u>\$154,446</u>	<u>\$177,043</u>	<u>\$173,370</u>	<b>\$-3.673</b>	<u>- 2.1%</u>

#### FY 1995 Accomplishments:

- O A better understanding of the thermal transformations of hydrocarbons is key to developing improved coal combustion and coal conversion technologies. A new semiempirical approach has been devised that quantitatively predicts needed thermochemical data for the important species involved in these thermal conversions.
- Basic studies have led to the identification of a new catalyst that can remove undesirable nitrogen oxides components from automobile exhaust as the auto is operated under highly fuel efficient conditions (lean-burn). Studies have shown that certain metal oxide-based catalysts, are active for the removal of the nitrogen oxides. Here, as in other research, the elucidation of the mechanism through identification of the reactive intermediates played a critical role.
- o Fundamental investigations of catalytic metal surfaces in the presence of carbon led to the realization that new carbide structures would be formed on iron surfaces at elevated temperatures in the presence of carbon-containing compounds. This led to the spin off discovery of a new high-temperature iron surface coating that has superior lubrication properties.
- o Laser pulses are used to study dynamical processes at ever shorter times. Basic combustion studies of the very short times required for a molecule to redistribute its energy or to fall apart at high temperatures led to a device which is now a commercial product to better characterize short laser pulses.
- The lack of general principles governing the relationship between catalytic activity and the physical, chemical, and electronic structure of the catalyst has impeded catalyst design for many energy intensive industrial applications. Recent catalysis basic research results have removed some of this impediment by showing how surface shape and structure have a major effect on catalytic activity.
- o New atomic physics experimental results on neutralization of ions through collisions with surfaces have improved our understanding of industrial plasma processes used for semiconductor electronics, materials strengthening and fusion technology.
- A technique developed to study combustion has been found to be broadly useful in experiments supported through other Federal programs. The method, photofragment imaging, has been used to identify a new path for the generation of ozone in the upper atmosphere. This result will help explain why current models underestimate the amount of ozone in the upper atmosphere.

- o A successful model of coal swelling in solvents is a significant advance that will permit improved coal conversion possibilities through better understanding of the structure-reactivity and chemical bonding relationships in coal.
- o Initiated realignment of a national laboratory radiation chemistry program into research critical to a better understanding of environmental issues associated with the remediation of tank wastes.
- A biomimetic system for photosynthesis has been developed that successfully mimics all of the properties of the natural photosynthetic protein. The system undergoes the necessary photochemical transformations with an efficiency that rivals the natural system and represents an important advance in the conceptual development needed for the conversion of solar energy into other energy forms.
- o Funding in the amount of \$3,169,000 and \$158,000 has been transferred to the SBIR and STTR programs, respectively.

#### FY 1996 Accomplishments (to date and planned):

- o Collaborative combustion related research critical to improved energy efficiency with reduced pollution in internal combustion engines and stationary combustors will be enhanced.
- o Research utilizing the major scientific user facilities will be enhanced in high priority research areas including combustion reaction dynamics, the characterization of environmental samples, materials precursors and plasma science for advanced processing.
- o Better integration of research in separations science, actinide chemistry, analytical chemistry and radiation chemistry will be carried out with those aspects closely related to environmental management programs and issues.
- o Separations research in support of analytical determinations and improved separation technology aimed at solving environmental problems will be emphasized.
- o Research on systems that mimic natural photosynthesis and offer a real opportunity for conversion of solar energy into other useful energy forms with minimal insult to the environment will be enhanced.

- New knowledge, both theoretical and experimental, of high and low temperature plasmas will be developed. These efforts will achieve a better physical and chemical understanding of the plasma so that technologies dependent upon such information will be improved.
- O Catalytic properties of roughened surfaces will be investigated to understand how the morphology of the roughened surface affects the selectivity of isomerization/hydrogenation reactions important to energy conversion and in nitric oxide decomposition reactions important to reducing emissions of environment pollutants associated with energy utilization.
- o Research will lead to new battery electrodes that will be transferred to the commercial sector for performance and scale up evaluation.
- o Funding in the amount of \$3,458,000 and \$259,000 has been budgeted for the SBIR and STTR programs, respectively.

#### FY 1997 Planned Accomplishments:

- o Research utilizing the major scientific user facilities will continue to be enhanced in high priority research areas including combustion reaction dynamics, the characterization of environmental samples, materials precursors and plasma science for advanced processing.
- o Interfacial chemistry research that emphasizes understanding of surface properties at the molecular level will provide new understanding of and improved catalytic and separations technologies.
- o Studies of the fundamental molecular properties of gases, liquids and solids will be carried out to aid development of molecularly selective separation processes.
- Theoretical advancements to resolve critical parameters in battery design and composition will be incorporated into new devices for evaluation of performance criteria.
- o Technical advances, building upon those from preceding years, will continue toward possible artificial high-efficiency photosynthetic devices that directly convert solar energy into chemical energy.

- o Laser-based diagnostics will be used to examine chemical processes involved in combustion. The systems to be examined will be isolated so as to gain fundamental understanding of the dynamics of the system which will be applied to actual combustion processes.
- o Synchrotron based atomic physics research will be applied to the study of atomic and plasma systems that will permit further advances in commercial plasma processes and fusion energy concepts.
- o Research in organic coal chemistry and analytical and radiation chemistry will be decreased.
- o Funding in the amount of \$4,334,000 has been budgeted for the SBIR program.

#### Explanation of Funding Changes FY 1996 to FY 1997:

Research in the areas of organic coal chemistry as well as analytical and radiation chemistry will be reduced (\$-2,867,000).

Overall operating time at user facilities such as NSLS, HFIR, CRF, REDC, and SSRL will be maintained at slightly below the FY 1996 level (\$-806,000).

## ENGINEERING AND GEOSCIENCES (Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives</u>:

This program conducts research in two disciplinary areas, Engineering and Geosciences, to support existing energy technologies and strengthen the foundation for future energy technologies. Ultimate research objectives include pollution avoidance, control, and remediation; increased energy efficiency; and assuring the underlying knowledge for the availability and responsible use of future energy supplies. The Engineering Research program serves as an effective conduit between basic science and applications-oriented research and development with the goals of maintaining technical leadership and stimulating job growth. Geosciences Research provides the foundation for environmentally sound, efficient, and economic use of the Earth's energy resources and provides a scientific foundation for innovative and efficient site characterization and remediation technologies. The Engineering and Geosciences research programs are implemented using individual investigator initiated research proposals subjected to merit (peer) review procedures.

#### II. Funding Schedule

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
Engineering Research	\$ 15,865	\$ 17,924	\$ 17,550	<b>\$-</b> 374	- 2.1%
Geosciences Research	18,770 \$ 34,635	20,887 \$ 38,811	23,700 \$ 41,250	+ 2,813 \$+ 2,439	+ 13.5% + 6.3%

#### FY 1995 Accomplishments:

Produced more than 300 publications in the peer-reviewed scientific literature dealing with research accomplishments in Engineering and Geosciences.

#### **Engineering**

- o Continued support for 36 three-year predoctoral fellowships addressing energy-related problems in integrated manufacturing.
- o Developed new insight into processes in flows of gas and liquids which has provided a better understanding of the onset of pulsating and irregular flow which causes damage in oil and gas pipelines.
- o Conducted theoretical and experimental studies which enable realistic models for prediction of the behavior of nonlinear systems with memory (i.e. hysteresis) occurring in most engineering systems and application (electrical motors/generators, chemical process plants, automobile tires, etc.).
- o Advanced the scientific basis for design and construction of autonomous intelligent systems (smart instruments, smart robots, smart sensors) for use in energy-related hostile environments (e.g. radioactive and mixed waste sites).
- o Performed studies on the effects of periodic and random temperature and stress changes on the reliability and longevity of energy structures.
- o Funding in the amount of \$325,000 and \$16,000 has been transferred to the SBIR and STTR programs, respectively.

#### Geosciences

o Developed new ways to observe small scale pore structure in rocks using laser scanning confocal microscopy and synchrotron-based high-resolution computed microtomography to improve foundation for predicting fluid (gas, oil, geothermal, ground water) flow and interaction in porous and fractured rocks.

- o Applied poroelasticity theory to observational data from a producing natural gas field to show the cause of microearthquakes and subsidence was volumetric contraction and very small (30MPa) stress changes associated with production.
- o Proposed an approach which can place an upper limit on the fractal scale dependence of mechanical and fluid transport properties of single fractures.
- O Collected and interpreted elemental, isotopic, and molecular data from natural samples to show that active migration of oil and gas to shallow reservoirs can take place rapidly (few years) showing that evaluation as a dynamic and replenishing system is essential.
- O Demonstrated that it is possible to use stable isotope information to trace multiple high-temperature geologic events in some zircons even in the presence of radiation damage.
- o Funding in the amount of \$383,000 and \$19,000 has been transferred to the SBIR and STTR programs, respectively.

#### FY 1996 Accomplishments (to date and planned):

#### **Engineering**

- o The first cohort (12) of National Academy of Engineering Department of Energy predoctoral fellows in energy-related integrated manufacturing will graduate.
- o Fundamental work on the behavior of dense suspensions and slurries will continue.
- o Nonlinear theories in mechanics will enhance the scientific basis for nonimaging optical systems, such as area illumination systems, energy efficient flat display screens for portable computers, etc.
- The feasibility of chemical sensors using in vitro samples of nerve tissue integrated with conventional electronics will be studied.

- o Research at the interface between chemical engineering and biology will continue to strengthen by providing the scientific basis for improving the practicality and economic viability of biological processes in energy-related applications.
- o Funding in the amount of \$350,000 and \$26,000 has been budgeted for the SBIR and STTR programs, respectively.

#### Geosciences

- o Initiate experiments on the GeoCARS beamline at the Advanced Photon Source (ANL) for space- and time-resolved spectroscopy providing unique information on mineral-fluid reactions important in energy and environmental applications.
- o Develop new methods of modeling and processing seismic data through collaborative basic research involving DOE Laboratory, University, and Industry researchers to obtain improved high-resolution, 3-D images of subsurface structure and properties.
- Obtain and interpret detailed images of subsurface electrical conductivity to assess role and magnitude of fluid flow in large-scale faulting and formation of fluid-filled reservoirs.
- O Continue research using partitioning of naturally occurring isotopes as tracers for mineral-fluid and gas-liquid reactions at spatial scales ranging from intragranular to sub-continental, as related to the origin, distribution, and recovery of energy resources.
- O Continue research on the role of sulfur/sulfonates, thermolytic decomposition of organic matter, and reactions between organic and inorganic rock constituents important in the origin, migration, and entrapment of oil, gas, geothermal fluids, and contaminated ground water.
- o Funding in the amount of \$410,000 and \$31,000 has been budgeted for the SBIR and STTR programs, respectively.

#### FY 1997 Planned Accomplishments:

#### **Engineering**

- o Second group of 12 National Academy of Engineering Department of Energy predoctoral fellowships will graduate and documentation of program effectiveness will be compiled.
- o Continue research at the forefront of the mechanical sciences with particular emphasis on the formation and dynamics of foams and the rheological behavior of suspensions and slurries.
- o Strengthen foundation for application of the theory of non-linear systems to improve the application to complex natural phenomena.
- o Continue research at a reduced level on interacting autonomous systems and reconfigurable systems which can readily adapt to changing tasks and environments.
- o Continue to strengthen research at the interface between biology and chemical process control to improve the practicality and viability of using biological processes in energy and environmental applications.
- o Research in engineering data and analysis will continue to provide critical thermodynamic data important for industrial processes and environmental cleanups, such as needed for separation of aqueous-hydrocarbon mixtures.
- o Funding in the amount of \$439,000 has been budgeted for the SBIR program.

#### Geosciences

- o Extend research in theoretical and computational modeling of atomistic-level reactions taking place at mineral-fluid surfaces using first principles methods and taking advantage of new data obtained at the Advanced Photon Source.
- o Refine high-resolution electromagnetic and seismic geophysical techniques for characterization of geologic structure and heterogeneity in fluid-bearing reservoirs of the Earth's upper crust using surface, surface to hole, and cross-hole methods.

- o Continue to develop integrated approach for analysis and interpretation of fracture-controlled fluid flow using advanced geophysical and rock mechanics methods with broad-based application to energy resource use issues.
- o Increase research on geochemistry, geophysics, and geohydrology of fluid flow and in sedimentary basins using integrated experimental, theoretical, and observational techniques.
- o Maintain research on fundamental physical, thermodynamic, and transport properties of rocks, minerals, geologic fluids and their synthetic analogues.
- o Funding in the amount of \$593,000 has been budgeted for the SBIR program.

#### Explanation of Funding Changes FY 1996 to FY 1997:

Funding will be reduced in the areas of intelligent control systems (\$-374,000).

Funding will be increased for basic research on fluid transport in, and geophysical imaging of, oil and gas reservoirs (\$+2,813,000).

#### **BASIC ENERGY SCIENCES**

#### **ENERGY BIOSCIENCES**

(Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives:</u>

The Energy Biosciences subprogram supports research to provide a basic understanding of the biological phenomena associated with the capture, transformation, storage and utilization of energy. The research on plant and non-medical microorganisms focuses on a range of biological processes including photosynthesis, bioenergetics, primary and secondary metabolism, the synthesis and degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of growth and development, thermophily and other phenomena associated with metabolism under harsh conditions. The research supported is fundamental and is selected to broadly support Department of Energy's goals and objectives.

#### II. <u>Funding Schedule:</u>

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
Energy Biosciences	<u>\$ 26,935</u>	\$ 28,700	<u>\$ 28,185</u>	<u>\$- 515</u>	<u>- 1.8%</u>
Total, Energy Biosciences	<u>\$ 26,935</u>	<u>\$ 28,700</u>	<u>\$ 28,185</u>	<u>\$- 515</u>	<u>- 1.8%</u>

#### III. <u>Performance Summary</u>:

#### FY 1995 Accomplishments:

- o Developed mutational strategies to study the synthesis of plant cell wall complex carbohydrates, the most abundant biopolymer.
- o First isolation of a gene that confers plant resistance to a bacterial disease provided new insights into the "immune" system of plants.

#### III. Performance Summary: ENERGY BIOSCIENCES (Cont'd)

- o Significant progress was made in elucidating the macromolecular structure, organization and catalytic mechanisms of the cellulose degrading complex from bacteria.
- o The biosynthetic pathway of an unusual fatty acid (petroselinic acid) was determined in oil seeds. Petroselinic acid has important chemical feedstock uses.
- o Demonstrated that individual enzymes from bacteria capable of living in the cold (psychrophilic bacteria) are active at significantly lower temperatures than their counterparts from temperate organisms.
- o Cover of recent <u>Science</u> magazine highlights "Emerging Plant Science." Of the five feature articles, three acknowledge Energy Bioscience support.
- o Funding in the amount of \$549,000 and \$28,000 has been transferred to the SBIR and STTR programs, respectively.

#### FY 1996 Accomplishments (to date and planned):

- o Enhance research activities examining the metabolism and physiology of extremely thermophilic (high temperature loving) bacteria.
- Studies on the metabolic capacities of plants to synthesize hydrocarbons and carbohydrates will be emphasized.
- o Continue to support graduate research training in specific sub-areas that will offer numerous future scientific and career opportunities.
- o Encourage new approaches to study the development and function of plant roots critical for the use of suboptimal/contaminated soils for bioresource production.
- o Biophysical and structural analyses of photosynthetic apparatus in plants and bacteria will continue to focus on establishing the precise molecular mechanisms involved.
- o Initiate studies on the role of membranes in bioenergetic conversions and transport.
- o Funding in the amount of \$562,000 and \$42,000 has been budgeted for the SBIR and STTR programs, respectively.

Performance Summary: ENERGY BIOSCIENCES (Cont'd)

#### FY 1997 Planned Accomplishments:

III.

- o Initiate genomic analysis of critical sections of the genetic material from the model plant, Arabidopsis.
- o Reduce activities focusing on describing molecular genetic regulatory strategies in plants and on the mechanisms involved in plant/pathogen interactions.
- o Microbial physiological studies will be augmented in order to continue to develop this underpopulated area and to take advantage of a number of new scientific opportunities.
- o Integrate knowledge of biochemical pathways to determine mechanisms regulating the overall flux of fixed carbon.
- o Initiate activities to determine the role of intracellular localization/compartmentalization on metabolic processes.
- o Funding in the amount of \$705,000 has been budgeted for the SBIR program.

#### **Explanation of Funding Changes FY 1996 to FY 1997**:

Research on the mechanisms involved in plant/pathogen interactions will be reduced along with studies aimed at describing molecular genetic regulatory strategies in plants (\$-515,000).

#### **BASIC ENERGY SCIENCES**

## RELATED CAPITAL FUNDING (Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives</u>:

The Related Capital Funding subprogram funds General Plant Projects (GPP), Accelerator and Reactor Improvements (AIP), and Capital Equipment in support of the BES research program.

#### II. <u>Funding Schedule:</u>

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
General Plant Projects (GPP)	\$ 11,412	\$ 6,415	\$ 9,275	\$+ 2,860	+ 44.6%
Accelerator and Reactor Improvements (AIP)	7,449	7,500	9,840	+ 2,340	+ 31.2%
Capital Equipment	<u>39,873</u>	<u>49,016</u>	<u>45,695</u>	<u>- 3,321</u>	- 6.8%
Total, Related Capital Funding	\$ 58.734	\$ 62.931	\$ 64.810	<u>\$+ 1.879</u>	+ 3.0%

#### III. Performance Summary:

#### FY 1995 Accomplishments:

- o Funding was provided for equipment in support of areas of high priority in the research programs, general purpose equipment requirements, and areas which required ES&H attention.
- o GPP funding was provided for minor new construction, other capital alterations and additions, and for buildings and utility systems. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may result in additions, deletions, and changes in the currently planned projects. The total estimated cost of each project will not exceed \$2,000,000.

#### Performance Summary: RELATED CAPITAL FUNDING (Cont'd)

o AIP funding supported additions and modifications to accelerator and reactor facilities which are supported by the BES research program.

#### FY 1996 Accomplishments (to date and planned):

III.

- Funding will be provided for equipment in support of areas of high priority in the research program, general purpose equipment requirements, and areas which required ES&H attention. Increased funding in support of the Advanced Photon Source and the User Facility Initiative.
- o GPP funding will be provided for minor new construction, other capital alterations and additions, and for buildings and utility systems. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may result in additions, deletions, and changes in the currently planned projects. The total estimated cost of each project will not exceed \$2,000,000.
- o AIP funding will support additions and modifications to accelerator and reactor facilities which are supported by the BES research program. The total estimated cost of each project will not exceed \$2,000,000.

#### FY 1997 Planned Accomplishments:

- Funding will be provided for equipment in support of areas of high priority in the research programs, general purpose equipment requirements, and areas which require ES&H attention. Decrease reflects reduced requirements in support of the Advanced Photon Source.
- o GPP funding will be increased for minor new construction, other capital alterations and additions, and for buildings and utility systems. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may result in additions, deletions, and changes in the currently planned projects. The total estimated cost of each project will not exceed \$2,000,000.
- o AIP funding will support additions and modifications to accelerator and reactor facilities which are supported by the BES research program.

#### III. Performance Summary: RELATED CAPITAL FUNDING (Cont'd)

#### Explanation of Funding Changes FY 1996 to FY 1997:

The reduction in capital equipment funding is due to decreased (\$-4,666,000) funding necessary to support the Advanced Photon Source and an increase (\$+1,345,000) in GPE for ORNL (\$-3,321,000).

GPP funding will be increased to support landlord responsibilities at Oak Ridge National Laboratory (\$+2,860,000).

The increase in AIP funding is due to the completion of one project over the \$2,000,000 threshold at LBNL in FY 1996. These funds are now included in the under \$2,000,000 category (\$+2,340,000).

#### **BASIC ENERGY SCIENCES**

#### CONSTRUCTION

(Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives:</u>

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

#### II. Funding Schedule:

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
Construction	\$ 58,379	\$ 9,986	\$ 11,500	\$+ 1,514	+ 15.2%
	\$ 58,379	\$ 9,986	\$ 11,500	\$+ 1,514	+ 15.2%

#### III. Performance Summary:

#### FY 1995 Accomplishments:

o Provided necessary funds to continue construction of the Advanced Photon Source at the approved schedule.

#### FY 1996 Accomplishments (to date and planned):

- o Complete funding of the Advanced Photon Source consistent with the approved schedule.
- o Provided the continued funding to complete (in 4 years) the Combustion Research Facility, Phase II.
- o Funding for Accelerator and Reactor Improvements and Modifications in excess of \$2,000,000 is provided for a liquid hydrogen cold source at the High Flux Isotope Reactor (HFIR) and an insertion device at the Advanced Light Source (ALS).

#### III. <u>Performance Summary</u>: CONSTRUCTION (Cont'd)

#### FY 1997 Planned Accomplishments:

- o Continue construction of the Combustion Research Facility, Phase II at the approved schedule.
- o Continue funding for construction of the Accelerator and Reactor Improvement (AIP) liquid hydrogen cold source project at the High Flux Isotope Reactor (HFIR).

#### Explanation of Funding Changes FY 1996 to FY 1997:

The increase (\$+1,514,000) is the net result of: completion of the Advanced Photon Source (\$-3,186,000); the scheduled increase in the construction of the Combustion Research Facility, Phase II (\$+7,000,000); and completion of the AIP project at LBNL (\$-2,300,000).



### MAJOR USER FACILITIES

(Tabular dollars in thousands, Narrative in whole dollars)

#### I. <u>Mission Supporting Goals and Objectives</u>:

The goal of the National User Facilities is to provide experimental capabilities which cannot otherwise be achieved in individual laboratories. These facilities are constructed and operated to support energy-related research, but are available to all qualified scientists based on the merit of their proposed experiments.

There were about 4,500 users in FY 1995 of Basic Energy Sciences-funded national user facilities. They conducted forefront research in materials, chemical, earth, biological, health, medical and other sciences. The costs for the construction and the environmentally acceptable and safe outside user-friendly operation of these world class facilities are substantially beyond the capability of the academic and private industrial sectors. The facilities are made available to all qualified users from the academic and private industrial sectors, and both DOE and non-DOE government laboratories. They thus permit the Nation's science and technology enterprise to have access to research instruments that are required for world-competitive cutting edge forefront research that would not otherwise be possible. All of the Basic Energy Sciences national user facilities have been constructed within cost, on schedule, and with rigorous compliance to all environmental, safety, and health regulations.

#### II. Funding Schedule: MAJOR USER FACILITIES (Cont'd)

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

Program Activity	FY 1995	FY 1996	FY 1997	\$ Change	% Change
		•			
National Synchrotron Light Source	\$ 23,491	\$ 26,599	\$ 26,915	<b>\$</b> + 316	+ 1.2%
High Flux Beam Reactor	21,100	23,732	24,060	+ 328	+ 1.4%
Intense Pulsed Neutron Source	6,800	10,867	10,970	+ 103	+ 0.9%
High Flux Isotope Reactor	24,248	26,925	27,165	+ 240	+ 0.9%
Radiochemical Engineering Development Center	7,070	7,234	7,310	+ 76	+ 1.0%
Stanford Synchrotron Radiation Laboratory	13,487	17,658	17,795	+ 137	+ 0.8%
Manuel Lujan, Jr. Neutron Scattering Center .	0	6,688	6,740	+ 52	+ 0.8%
Combustion Research Facility	4,171	4,402	4,445	+ 43	+ 1.0%
Advanced Light Source	21,200	28,616	28,945	+ 329	+ 1.1%
Advanced Photon Source	64,771	78,671	80,000	+ 1,329	+ 1.7%
Undesignated	1,304	5,115	0	<u>- 5,115</u>	<u>-100.0%</u>
Total, Major User Facilities	<u>\$ 187,642</u>	<u>\$ 236,507</u>	<u>\$ 234,345</u>	<u>\$- 2,162</u>	- 0.9%

#### FY 1995 Accomplishments:

- Thousands of experiments have been carried out on the various unique synchrotron beam lines that are dedicated to myriad experiments of importance to many disciplines at the National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory and the Advanced Light Source. They have provided progress in the understanding of catalysis and surface reactions, chemical bond characterization, the atomic structure of materials, trace chemical analysis as well as the structure of highly charged atomic ions.
- o Commissioning of the Advanced Photon Source Storage Ring has begun and a circulating current of 8.5 milliamperes was achieved resulting in the first x-ray beams at this third generation x-ray source. The design current is 100 milliamperes.

#### III. Performance Summary: MAJOR USER FACILITIES (Cont'd)

- Experiments for the characterization of residual stress in manufactured parts, crystalline structure and excitation of solids such as high temperature superconductors, magnetic materials, neutron radiation damage, materials important in structural biology and hydrogen containing materials such as polymers, were carried out at the High Flux Beam Reactor and the High Flux Isotope Reactor.
- o Several new beamlines, insertion devices and specialized end stations are being developed for implementation at the Advanced Light Source and the Advanced Photon Source.
- The narrow-gap undulator concept was successfully tested at the National Synchrotron Light Source, which will enhance the energy range which can be provided to users at NSLS.
- Tests of a prototype commercial gas burner at the Combustion Research Facility has led to improved design of a low NO<sub>x</sub> emission burner.

#### FY 1996 Accomplishments (to date and planned):

- The existing National User Facilities will operate more effectively (in some cases with substantial increases in operating hours, and in others, with the implementation of modern state-of-the-art instrumentation which will use the neutron and photon beams more effectively) with more experiments and more users as a consequence of the President's User Facility Initiative.
- Thousands of experiments will be carried out on the various unique synchrotron beam lines that are dedicated to myriad experiments at the National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory and the Advanced Light Source. The first experiments will be carried out on the Advanced Photon Source.
- o Experiments for the characterization of residual stress, magnetic structure and excitations, neutron irradiation damage and hydrogen containing materials will be carried out at the High Flux Beam Reactor and the High Flux Isotope Reactor.
- o Additional beamlines will be implemented at the Advanced Light Source and the Advanced Photon Source.

  Instrumentation at NSLS, SSRL, IPNS, HFBR and HFIR will be upgraded. LANSCE will resume operations.

#### III. Performance Summary: MAJOR USER FACILITIES (Cont'd)

#### FY 1997 Planned Accomplishments:

- o The National User Facilities will continue to operate much more effectively with more experiments and more users as a consequence of the President's User Facility Initiative which will be sustained in FY 1997.
- o Beamlines at the National Synchrotron Light Source and the Stanford Synchrotron Radiation Laboratory will be upgraded with modern state-of-the-art instrumentation to make more effective use of these unique x-ray sources.
- o Operation of the Advanced Photon Source will be initiated.
- o New beamlines will be built at the Advanced Light Source and the Advanced Photon Source in FY 1997 including insertion devices to produce circularly polarized x-ray beams.
- Advanced experiments for the characterization of residual stress, magnetic structure and excitations, neutron irradiation damage and hydrogen containing materials will be carried out at the High Flux Beam Reactor and the High Flux Isotope Reactor.

#### Explanation of Funding Changes FY 1996 to FY 1997:

Overall operating time at user facilities will be maintained at slightly below the FY 1996 level (\$-2,162,000).

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

		FY 1995	FY 1996	FY 1997	\$ Change	% Change	
Capital Oper	ating Expenses				,		
General Pla	nt Projects (total)	\$11,412	\$6,415	<b>\$</b> 9,275	\$+2,860	+44.6%	
	22 million (total)		7500	9,840	+2,340	+31.2%	
Capital Equ	ipment (total)	39,873	49,016	45,695	-3,321	-6.8%	
Construction	Project Summary (both Operating and Construction Fu	nded)					
		·					
Project No.	Project Title		Previous	FY 1995	FY 1996	FY 1997	Unapprop.
-	•	TEC	Appropriated	Appropriated	Appropriated	Request	Balance
97-E-305	Accelerator and Reactor Improvements & Modifications, Various Locations						
96-E-300	Combustion Research Facility, Phase II, SNL	\$2,500	\$0	\$0	.\$4,800	\$2,500	\$0
89-R-402	6-7 GeV Synchrotron Radiation Source, ANL	26,800	4,800	0	2,000	9,000	11,000
Total Basic I	Energy Sciences	467,178	405,613	58,379	3,186	0	0
		\$XXXXX	\$410,413	\$58,379	\$9,986	\$11,500	\$11,000
Detailed Brea	January.						
Detailed Die	akouts	T-4-1	D	ES 1006	EV 1006	EV 1007	11
CDD1. F-		Total	Previous	FY 1995	FY 1996	FY 1997	Unapprop.
	eeding \$3 million	CDR Cost	Appropriated	Appropriated	Appropriated	Request	Balance
1. Puised 3	Spallation Neutron Source						

\$15,635

\$7,635

\$8,000

## DEPARTMENT OF ENERGY FY 1997 CONGRESSIONAL BUDGET REQUEST

## ENERGY SUPPLY, RESEARCH AND DEVELOPMENT (Tabular dollars in thousands. Narrative material in whole dollars.)

#### **Basic Energy Sciences**

1. Title and Location of Project:	Accelerator and Reactor Improvements	2a.	Project No. 97-E-305	
	and Modifications, various locations	<b>2b</b> .	Construction Funded	
3a. Date A-E Work Initiated, (Title I	Design Start Scheduled): 1st Qtr. FY 1996	5.	Previous Cost Estimate: None	<del></del>
			Total Estimated Cost (TEC): None	
3b. A-E Work (Title I & II) Duration	: Months vary per project		Total Project Cost (TPC): None	
4a. Date Physical Construction Starts:	3rd Qtr. FY 1997	6.	Current Cost Estimate:	
			TEC \$ 2,500	
4b. Date Construction Ends: 3rd Qtr.	FY 1999		TPC \$ 2,500	

## 7. <u>Financial Schedule</u>: (Federal Funds)

Fiscal Year	<b>Appropriation</b>	<b>Obligations</b>	Costs
1997	\$ 2,500	\$ 2,500	\$ 1,500
1998	0	0	1,000
1999	0	0	0

1.

Title and Location of Project: Accelerator and Reactor Improvements

Project No. 97-E-305 2a.

and Modifications, various locations

2b. Construction Funded

#### Project Description, Justification and Scope 8.

This project provides for additions and modifications to accelerator and reactor facilities, which are supported by the Basic Energy Sciences program. Since program priorities and needs change, the projects described below indicate the most likely projects to be funded.

The following are the projected items of work to be performed at the various locations. Since needs and priorities may change, other projects may be substituted for the examples listed below, and some of these may be located on non-Government owned property.

High Flux Isotope Reactor (ORNL)

\$ 2,500

Install a liquid hydrogen cold source in an existing beam port at the High Flux Isotope Reactor (HFIR). The cold source will provide a cold neutron brightness as good or better than that of the Institute Laue Langevin, the world's premier cold neutron facility. The proposed HFIR facility will provide the United States with unsurpassed capabilities in this rapidly expanding area of neutron sciences. The estimated cost to design, construct and install the cold source is \$5,000,000, \$2,500,000 in FY 1996 and \$2,500,000 in FY 1997.

#### 9. **Details of Cost Estimate**

Engineering, design, and inspection and component assembly a. and installation

\$ 2,500

Total line item cost \$ 2,500

#### Method of Performance 10.

Design, engineering and inspection will be performed by Oak Ridge National Laboratory. To the extent feasible, construction and procurement will be accomplished by fixed-price contracts and subcontracts awarded on the basis of competitive bidding.

### DEPARTMENT OF ENERGY

#### FY 1997 CONGRESSIONAL BUDGET REQUEST

(Changes from FY 1996 Congressional Budget Request are denoted with vertical line in left margin)

#### ENERGY SUPPLY, RESEARCH AND DEVELOPMENT

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

#### **Basic Energy Sciences**

	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a. 2b.	Project No. 96-E-300 Construction Funded
,	Date A-E Work Initiated, (Title l	Design Start Scheduled): 1st Qtr., FY 1988	5.	Previous Cost Estimate:
	A-E Work (Titles I & II) Duration: 12 months			Total Estimated Cost (TEC) None Total Project Cost (TPC) None
	Date Physical Construction Starts	s: 4th Qtr., FY 1988	6.	Current Cost Estimate: TEC \$26,800
	Date Construction Ends: 4th Qt	., FY <sup>.</sup> 1999		TPC \$30,020

## 7. Financial Schedule: (Federal Funds)

Fiscal Year	<b>Appropriation</b>	<b>Obligations</b>	Costs
Prior Years	a/ \$ 4,800	\$ 4,800	\$ 4,205
1995	0	0	4
1996	2,000	2,000	1,700
1997	9,000	9,000	9,400
1998	7,000	7,000	6,800
1999	4,000	4,000	4,691

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

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

#### 8. Project Description, Justification and Scope

Phase II of the Combustion Research Facility (CRF) will add approximately 32,300 gross square feet to the existing 51,100 square-foot multibuilding CRF facility (Project No. 78-13-B, TEC \$9.4 million) at Sandia National Laboratories, Livermore (SNL/L). Phase II will add 21,200 square feet to the existing 16,400 square-foot laboratory building and 11,100 square feet to the existing 25,000 square-foot office building. The project will include such site modifications and improvements as yard paving, walkways, landscaping, fencing, signage, and east entrance road relocation.

The project has been delayed due to budget constraints from FY 1989 through FY 1995. The appropriations totaling \$4.8 million in FY 1987 and FY 1988 were used for site preparation and design and construction of the shell of the laboratory building addition. The appropriations in FY 1996-FY 1999 will complete the balance of the project.

The laboratory building addition will be an L-shaped extension to the south and east of the existing building. Construction of the addition will match the existing building in architectural style, materials, and finishes, color, and floor-to-floor heights. The laboratory building addition will provide sixteen new laboratory spaces and two facility laser laboratories. The new facility laser rooms will be connected to serve any Lab in the facility, via the Laser Duct and Periscope System.

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

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

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

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

#### 8. Project Description, Justification and Scope (Continued)

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

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

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

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

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

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

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

#### 8. Project Description, Justification and Scope (Continued)

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

There is a continuing need for the CRF to advance combustion-related science and technology to a higher level. The improvements included in the Phase II project will address this need. For example, special lasers and equipment will be developed to provide the ability to measure quantitatively entire two- and three-dimensional images of a system's physical and chemical properties with better resolution, and far greater speed than is now possible. It is this type of advance in the science of combustion that will allow the pursuit of the increasingly more difficult and complex problems that face our country.

CRF Phase II will enable attacking many complex problems directly associated with combustion. An important example is the need for improved combustion processes that incorporate high efficiency together with minimum production of pollutants such as NO<sub>x</sub> and air toxics. Rapid progress on these problems both in engines and in furnaces requires Phase II's next-generation diagnostic capabilities. Completion of Phase II will also enable using the tools and expertise developed in Phase I to address broader challenges facing the country. CRF basic research in laser diagnostics, for example, will underpin remote sensing applications that contribute to global-change research and to nonproliferation of weapons. Basic research in chemically reacting flows will continue to support improved U.S. competitiveness in semiconductor processing and will support the development of new industrial materials. Basic research in chemistry will address new processes, such as supercritical water oxidation, for destroying hazardous wastes with minimal environmental impact.

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

			·_		
1.	Title and Location of Project:	Combustion Research Facility, Phase II	2a.	Project No. 96-E-300	
		Sandia National Laboratories Livermore, California	<b>2</b> b.	Construction Funded	
		Divermere, Camorna		•	

#### 8. Project Description, Justification and Scope (Continued)

The normal increase in both the quantity and sophistication of combustion research by Sandia staff, together with the heightened requirements of visiting scientists, have completely saturated the facilities provided under CRF Phase I. During the past ten years the number of scientists who visit the CRF long enough to participate in research has almost tripled. In fiscal year 1993 forty professional staff hosted eighty nine such visits. Many important experiments cannot be carried out in the existing facilities because of a lack of space. Access to the unique capabilities of the CRF (such as the Facility lasers and computer resources) is essential for studying trade-offs between combustion efficiency and the pollution that results from existing and alternative fuels. However, much of the combustion research and diagnostics development work at Sandia is currently being done in facilities that are widely scattered throughout Sandia/CA where the researchers do not have access to these unique capabilities. Additional laboratories will permit the consolidation of these experiments at the CRF, thus providing the necessary access to the unique capabilities at the Facility. It will also provide adequate space and ready access to visiting scientists.

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

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

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

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

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

The \$9 million of FY 1997 funds will be used in part for completing project management, construction management, and inspection of the 11,100 square foot office addition. The remainder of the funds will be used to complete design, place a construction contract, and initiate construction for the 21,200 square foot laboratory expansion and mechanical building modification.

Deta	ils of Cost Estimate	Unit Cost	Item Cost	Total Cost
a.	Engineering, design, and inspection (ED&I)			\$3,100
	1. Engineering, design, and inspection at approximately 15 percer	nt of		
	construction		2,050	
	2. Construction management costs		500	
	3. Project management		550	
b.	Construction costs	•		14,610
	1. Improvements to land		1,010	
	Paving, walkways, landscaping, fencing, signage, road relocation parking lot rearrangement	on		
	2. Buildings		12,800	•
•	(a) Office Building (11,000 SF \$190/SF)	2,300		
	(b) Laboratory Building (21,200 SF \$415/SF)	9,740		
	(c) Mechanical Building (Existing)	760		
	3. Utilities		800	
	Water, sanitary sewer, natural gas, site lighting, electrical power, signal systems			
C.	Standard equipment		•	5,450
	Lasers, spectrometers, analyzers, processing equipment			
	Subtotal			23,160
d.	Contingency at approximately 16 percent of above costs			3,640
1	Total line item cost	290		\$ \$ 300

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

#### 9. Details of Cost Estimate: (Continued)

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

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

#### 10. Method of Performance

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

#### 11. Schedule of Project Funding and Other Related Funding Requirements

	Prior				•	
	<b>Years</b>	FY 1995	FY 1996	FY 1997	FY 1998	FY 1999 Total
a. Total project funding	•			•		•
1. Total facility costs	•					
(a) Line item	<u>\$4,205</u>	<u>\$_4</u>	<u>\$1,700</u>	<u>\$ 9,400</u>	<u>\$ 6,800</u>	<b>\$4,691 \$26,800</b>
Total direct cost	4,205	4	1,700	9,400	6,800	4,691 26,800
2. Other project costs						٠.
(a) Other project costs	220	0	0	500	750	750 2,220
(b) Capital equipment	0	0	0	500	<u>250</u>	<u>250</u> <u>1,000</u>
Total other project costs.	220	0	0	_1,000	<u>1,000</u>	<u>1,000</u> <u>3,220</u>
Total project cost (TPC)	\$4,425	\$ 4	\$1,700	\$10,400	\$ 7,800	\$5,691 \$30,020

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

#### 11. Schedule of Project Funding and Other Related Funding Requirements (Continued)

b.	Related annual costs a/ (estimated life of building: 50 years)	
	1. Facility operating costs	\$ 300
	2. Programmatic operating expenses directly related the facility	2,400
	3. Capital equipment not related to construction but related to the programmatic	
	effort in the facility	400
	4. GPP or other construction related to programmatic effort in the facility	200
٠	5. Other costs	0
	Total related annual costs	\$ 3,300

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

- a. Total project costs:
  - 1. Total facility costs
    - (a) Construction Line Item as described in previous items.
  - 2. Other project costs
    - (a) Other project costs \$220,000 of operating funds have been paid to architect engineering firms for preparation of conceptual designs/conceptual design reports and supplemental information for this project. \$500,000 in FY 1997, \$750,000 in FY 1998, and \$750,000 in FY 1999, are operating costs associated with the new facility.
    - (b) \$500,000 in FY 1997, \$250,000 in FY 1998, and \$250,000 in FY 1999 is for capital equipment associated with the new facility.

Estimated costs in thousands escalated to 1999-year dollars. The related annual funding displayed is related to CRF, Phase II project only. These amounts are in addition to annual funding for the existing CRF operations (\$4,739,000 in the FY 1997 OMB Budget Request).

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

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

- b. Related annual costs:
  - 1. Facility operating costs

    This cost represents the annual operating expenses for utilities, maintenance, and janitorial service incurred due to the increase of 32,300 gross square feet in laboratory and office space.
  - 2. Programmatic operating expenses
    Staff increase resulting from this project is estimated to be six people. Costs also include acquisition of computer resources that will serve both resident staff and visiting scientists.
  - 3. Capital equipment not related to construction

    The increase in annual capital equipment is estimated at \$400,000. This is in addition to Capital Equipment funds currently allocated to the CRF.
  - 4. Maintenance, repair, GPP or other construction related to programmatic effort
    The annual GPP needs for Phase II are expected to be approximately \$200,000. This is in addition to GPP funds presently allocated to the CRF.
  - Other costs
     No other costs are anticipated.