Office of Science

Basic Energy Sciences

Core Research Activities

May 2006

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Mechanical Behavior of Materials & Rad Effects
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Physical Behavior of Materials
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🟩 Jeffrey Tsao, SNL
◆ Daniel Friedman, NREL

Engineering Research
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Condensed Matter Phys and Materials Chemistry X-Ray & Neutron Scat.

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🟩 Doug Finnemore, Ames

Theoretical Condensed Matter Physics
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Materials Chemistry & Biomolecular Materials
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Altaf (Tof) Carim

Spallation Neutron Source (Construction)
Jeffrey Hoy

Nanoscale Science Research Centers (Construction)
Altaf (Tof) Carim
◆ Tom Brown, ANL

Linac Coherent Light Source (Construction)
Jeffrey Hoy

Instrument MIEs (SNS, LCLS, etc.)
Jeff Hoy
◆ Tom Brown, ANL

NSLS II
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◆ Tom Brown, ANL

Chemical Sciences, Geosciences, and Biosciences Division

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Fundamental Interactions

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Robin Felder, Prg Asst

Atomic, Molecular, and Optical Science
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Chemical Physics
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▲ Frank Tully, SNL

Photochemistry & Radiation Research
Mary Gress
◆ Mark Spitler, NREL

Computational and Theoretical Chemistry
Richard Hilderbrandt

Molecular Processes and Geosciences

John Miller
Vacant, Prg Asst

Catalysis and Chemical Transformation
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Paul Maupin
◆ Michael Chen, ANL

Separations and Analysis
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Heavy Element Chemistry
Lester Morss
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Chemical Energy and Chemical Engineering
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Plant Sciences Biochemistry and Biophysics
Richard Greene
◆ Michael Kahn, PNNL
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▲ IPA
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🟩 Detailee, 1/4 time, not at HQ

April 2006

Research Activity: **Atomic, Molecular, and Optical Sciences**
Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact(s): Michael P. Casassa (E-Mail: Michael.Casassa@science.doe.gov; 301 903-0448)
Team Leader: Eric Rohlfing
Division Director: Eric Rohlfing (Acting)

Portfolio Description:

The Atomic, Molecular, and Optical Sciences (AMOS) activity supports basic research on fundamental interactions among atoms, molecules, electrons, and photons. The program supports experiments and theory to understand and control: ultrafast interactions of intense electromagnetic fields with atoms and molecules; correlated many-body interactions in systems far from equilibrium; novel chemical and emergent phenomena in ultracold ensembles of atoms and molecules; and light-matter interactions on the nanometer scale. The activity strongly supports development and application of novel x-ray light sources and ultrafast probes to enable future research in the chemical sciences and to enable research at current and planned BES user facilities. By studying the fundamental interactions among atoms and molecules, AMOS provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer between molecules and ultimately the making and breaking of chemical bonds.

Unique Aspects:

The knowledge and techniques developed in the AMOS activity underpin other fundamental science efforts of the Department of Energy (DOE), including research conducted at BES user facilities, as well as having wide applicability in enabling science and technology. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, enhancing our ability to understand materials of all kinds and enabling full exploitation of the BES x-ray sources and Nanoscale Science Research Centers (NSRCs). This enabling aspect will continue to be emphasized, particularly with respect to research into the generation and application of ultrashort, intense x-ray pulses. The AMOS activity includes ultrashort x-ray pulse generation and applications at the Advanced Light Source (ALS) and Advanced Photon Source (APS), and it is the major supporter of synchrotron-based AMO science in the United States. The AMOS program continues its role as the principal U.S. supporter of research into the properties and interactions of highly charged atomic ions, which is of direct consequence to fusion plasmas.

Relationship to Other Programs:

The AMOS program supports current and planned experiments concerning x-ray characterization and AMO science at the Sub-Picosecond Photon Source (SPPS) and the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC), in coordination with the BES Scientific User Facilities Division. The AMOS program funds research at the new Ultrafast Science Center at SLAC which is supported by the BES Materials Sciences and Engineering Division. The AMOS activity co-funds with the BES Condensed Matter Physics activity an ultrafast x-ray beamline at the ALS. Numerous complementary relationships exist between AMOS program elements and other core research activities across the BES Chemical Sciences, Geosciences, and Biosciences Division. Fundamental insight and data obtained in the AMOS activity are relevant to Office of Fusion Energy Sciences (FES) programs in atomic data for fusion modeling and basic plasma physics. This synergy is notable at the Multicharged Ion Research Facility (MIRF) at Oak Ridge National Laboratory (ORNL), which is co-funded by BES and FES. The AMOS program also elucidates interactions of intense laser fields with high-energy plasmas which are relevant to defense programs in DOE. A close working relationship exists with the National Science Foundation (NSF) Atomic, Molecular, Optical and Plasma Physics Program, and these two program are co-funding the National Academy of Sciences/National Research Center Physics Decadal Survey, *"AMO 2010: An Assessment of and Outlook for Atomic, Molecular, and Optical Science."* In FY 2005, the AMOS Program provided partial support for the 10th International Conference on Multiphoton Processes (ICOMP2005) and the 2005 Gordon Conference on Atomic Physics.

Significant Accomplishments:

The AMOS activity has been a major U.S. supporter of experimental and theoretical studies of the fundamental properties of atoms, ions, and small molecules and of collisional interactions between atoms, ions, molecules, and surfaces. This has produced a vast knowledge base on the properties of atoms, ions, and small molecules, with a broad impact on science and technology. It has led to the development of powerful new methods for momentum imaging of collision fragments that have seen wide application in atomic, molecular, and chemical physics. The knowledge is now being used to manipulate the quantum behavior of atoms and molecules and has propelled further development and scientific applications of ultrafast x-ray sources using table-top lasers and 3rd generation synchrotrons (ALS and APS). Enhanced high-harmonic generation (HHG) using quasiphase matching and ionized atoms for soft x-ray production has been demonstrated, and fundamental interactions of intense controlled laser fields with atoms and small molecules leading to ionization and fragmentation have been explored. Recent efforts involving high-field interactions, ultrafast processes, and ultrashort x-ray pulses are creating the science base required for the research that will be done at 4th generation light sources like the LCLS. Highlights from the past year include: detailed measurements and exact computations to understand the molecular breakup triggered by absorption of hard x-ray photons, such as will be prevalent with 4th-generation x-ray sources; observation of carrier multiplication in nanocrystals by which single photons produce multiple charge carriers, possibly providing a path toward more efficient solar energy conversion; observation of superfluidity in an ultracold Fermi gas of atoms, which may provide insight into other strongly interacting systems of particles such as the electrons in high T_C superconductors; and recognition of international scientific leadership by AMOS-sponsored investigators through MacArthur, Rabi, Goeppert-Mayer, Davisson-Germer awards, American Physical Society Fellowships, and National Academy memberships.

Mission Relevance:

AMO science underpins a wide spectrum of DOE research activities and lays the scientific foundation for research performed at BES scientific facilities. New ways to control and probe interactions in the gas and condensed phases enhance our ability to understand materials of all kinds and enable the full exploitation of the BES x-ray sources and NSRCs. The study of intense field and ultrafast x-ray interactions provides a basis of understanding essential for experiments anticipated at 4th generation light sources. The research on many-body phenomena addresses issues of chemical reactivity important to DOE including electron-driven processes relevant to radiation chemistry and reactions of ions and other species important to fusion plasmas. Research on ultracold atoms and molecules explores regimes of behavior and control that are inaccessible under normal conditions, enabling careful manipulation and investigation of long-range cooperative effects, complex interactions, and emergent phenomena. The research to understand nanoscale light-matter interactions underpins research in photo-energy conversion relevant to the use of solar energy, enables the development scientific tools for nanoscale materials characterization and chemical imaging, and advances our ability to study and control the properties of matter and chemical reactivity on the nanometer scale. Thus AMOS contributes at the most fundamental level to the science-based optimization of current energy sources and the development of new ones.

Scientific Challenges:

In recent years, AMO science has seen a transformation; it has changed from a field in which the fundamental interactions of atoms, molecules, photons, and electrons are probed to one in which they are controlled. Systems studied are increasingly complex. Correlated, non-perturbative interactions are the norm. AMOS practitioners can now shape the quantum mechanical wavefunctions of atoms and small molecules using controllable laser fields; trap and cool atoms and molecules to temperatures near absolute zero where cooperative phenomena can be precisely controlled; create nanoscale structures which manifest novel light-matter interactions and properties; and coherently drive electrons in atoms, plasmas, or synchrotron orbits to generate ultrafast x-ray pulses. These capabilities create opportunities to investigate chemical processes under conditions which are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
16,627	15,397	19,248

Performer	Funding Percentage
DOE Laboratories	39 %
Universities	60 %
Other	1 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

The activity provides funding for 55 university grants partially supporting about 60 faculty and senior staff. It also funds 4 programs at national laboratories supporting about 20 senior staff. Programs at the laboratories are multi-investigator efforts focusing on problems that require extensive participation by senior scientists and postdoctoral associates. These programs underscore unique facilities at the DOE national laboratories, including the MIRF at ORNL, the ALS at Lawrence Berkeley National Laboratory (LBNL), and the APS at Argonne National Laboratory (ANL). A program at Los Alamos National Laboratory (LANL) on optical properties of semiconductor nanocrystals is strongly affiliated with the new Center for Integrated Nanotechnologies at LANL and Sandia National Laboratories (SNL). The activity supports the J. R. MacDonald Laboratory at Kansas State University, a multi-investigator program devoted to the experimental and theoretical study of intense-field physics produced either by ultrafast lasers or collisions with highly charged ions.

Projected Evolution:

The AMOS activity will continue support for AMO science that advances DOE and BES mission priorities. Closely related experimental and theoretical efforts will be encouraged. AMOS will continue to have a prominent role in at BES facilities in understanding the interaction of intense, ultrashort x-ray pulses with matter; in the control and investigation of light-matter interactions with nanoscale structures; and in the investigation of ultrafast processes. Key targets for greater investment include: ultrafast electron diffraction; attosecond physics with phase-controlled pulses; electron-driven processes; quantum control for molecular processes; ultracold molecular interactions, and nonlinear optics relevant to ultrafast, short wavelength, and nanoscale physics.

The program will strongly emphasize ultra-fast, ultra-intense, and short-wavelength science. The development and application of novel x-ray light sources using existing synchrotrons or table-top lasers will continue. Topics of interest include the development of high-harmonic generation or its variants as soft x-ray sources, development and characterization of femtosecond pulses of x-rays at existing synchrotrons and new accelerator-based sources, and applications in the chemical and materials sciences. Coherent control of nonlinear optical processes and tailoring quantum mechanical wavefunctions with lasers will grow in importance, particularly in chemical systems.

Opportunities include theory and experiment for artificial nano structures in materials and their interactions with light, and the use of nonlinear spectroscopies to characterize the optical properties of nanoscale systems. Opportunities also include the creation of ultracold ensembles of atoms and molecules to investigate and control long range cooperative or emergent phenomena and chemical interactions under these conditions.
Fundamental studies of highly charged ions and their interactions with atoms, molecules, and surfaces will continue to further develop the knowledge base important to fusion plasmas. Opportunities include the use of the experimental and theoretical AMOS tools in the study of low-energy electron-molecule interactions in the gas and condensed phases.

Research Activity: Chemical Physics Research

Division: Chemical Sciences, Geosciences, and Biosciences
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Team Leader: Eric A. Rohlfing
Division Director: Eric A. Rohlfing (Acting)

Portfolio Description:

This activity supports experimental and theoretical investigations in the gas phase, in condensed phases, and at interfaces aimed at elucidating the chemical and physical interactions that govern combustion, surface reactivity, and solute/solvent structure, reactivity, and transport. Gas-phase chemical physics research emphasizes studies of the dynamics and rates of chemical reactions at energies characteristic of combustion and the chemical and physical properties of key combustion intermediates. The overall aim is the development of validated theories and computational tools for predicting chemical reaction rates for use in combustion models and experimental tools for validating these models. Combustion models using this input are developed that incorporate complex chemistry with the turbulent flow characteristic of real combustion processes. The surface, interfacial, and condensed-phase chemical physics portion of this activity is focused in two areas. The study of chemistry at well characterized surfaces and the reactions of metal and metal-oxide clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target a first-principles understanding of molecular reactivity in solution and at interfaces; often, this approach confronts the transition from molecular-scale chemistry to collective phenomena in complex systems.

Unique Aspects:

The Department of Energy (DOE) is the largest supporter of basic research in combustion in the federal government. This program is the principal supporter of high-temperature chemical kinetics and gas-phase chemical physics in the nation. This activity also has oversight for the Combustion Research Facility (CRF), a BES user facility for the study of combustion science and technology. In-house BES supported efforts at the CRF combine theory, modeling, and experiment including diagnostic development, chemical kinetics, and simulations of reactive, turbulent flows. Several innovative non-intrusive diagnostics are being developed to characterize gas-phase processes, including high-resolution optical spectroscopy, time-resolved Fourier transform infrared spectroscopy, picosecond laser-induced fluorescence, and photoionization mass spectrometry using tunable synchrotron radiation. Benchmark numerical simulations of turbulent combustion are conducted on Office of Science leadership class platforms and a CRF mid-range computing cluster. The CRF provides outreach and organization to the broader combustion community through activities such as the semi-annual, turbulent non-premixed flame (TNF) workshop. Interactions with the Office of Fossil Energy (FE), the Office of Energy Efficiency and Renewable Energy (EERE), and industry are enhanced at the CRF through the co-location of their applied research projects with BES-supported fundamental research.

The surface chemistry work in this activity focuses on identifying, characterizing, and manipulating individual reactive sites on surfaces or clusters of relevance to heterogeneous catalysis, providing an underpinning for work supported in the BES Catalysis and Chemical Transformations activity. The condensed phase and interfacial research on electron-driven processes and reaction dynamics in this activity is relevant to chemistry initiated by ionizing radiation that is studied within the BES Photochemistry and Radiation Research activity. Solute/solvent dynamics and transport phenomena studied in this activity are well connected to DOE mission needs in the area of waste remediation, particularly through the experimental and theoretical condensed phase chemical physics programs at Pacific Northwest National Laboratory.

The Scientific Discovery through Advanced Computing (SciDAC) thrust within the chemical physics program addresses two fundamental application software development efforts: (1) chemically reacting flows and (2) the chemistry of unstable species and large molecules. Each of these efforts is carried out by a team of related scientists working with the appropriate Integrated Software Infrastructure Centers supported under SciDAC by the Office of Advanced Scientific Computing Research within the Office of Science.

Relationship to Other Programs:

Combustion research is also conducted under various research programs within EERE and FE. Linkages with this program vary in formality. In addition, combustion-related chemical physics research is conducted by the Air Force Office of Scientific Research (AFOSR), Office of Naval Research (ONR), Army Research Office (ARO), National Aeronautics and Space Administration (NASA), National Institute of Standards and Technology (NIST), and National Science Foundation (NSF). The AFOSR and NASA programs support research in propulsion. NASA and NIST programs investigate fire propagation. ONR and ARO research focuses on organic waste remediation. NSF supports basic research. Surface science is supported through several federal programs, both applied and basic.

Significant Accomplishments:

Within the last ten years, theories and computer codes for the calculation of chemical properties and, in particular, chemical reaction rates, have achieved a high degree of accuracy and reliability for systems of a few atoms. The theoretical developments have been inspired and validated by nearly a quarter of a century of molecular beam, spectroscopy, dynamics, and kinetics research on the detailed measurement of reactions as functions of collision energy and internal energies of reactants and products. Research in the Chemical Physics program has played a prominent role in this development. Professor Y. T. Lee, one of three recipients of the 1986 Nobel Prize in Chemistry for molecular-beam chemical dynamics research, was supported by the Chemical Physics program for his entire U.S. research career. Continuing laser-based experimental research and computationally intensive theoretical work provide the fundamental basis for developing a predictive capability for chemically reacting flows.

Mission Relevance:

The molecular-level studies in this activity are motivated by energy security, environmental preservation, and new opportunities fostered by a predictive understanding of chemical reactivity. Since 85 percent of nation’s energy use is derived from burning fossil fuels, the gas-phase portfolio strives to acquire the fundamental information necessary to develop predictive combustion models. Such models are required for optimal design and operation of next-generation combustion and pollution-abatement devices so as to maximize energy efficiency and minimize deleterious impact on the global environment. This thrust complements the more applied combustion programs in FE and EERE. The chemical physics program supports the development of theories and computational algorithms to predict the rates of chemical reactions at temperatures characteristic of combustion. It supports the development and application of experimental techniques for characterizing gas-phase reactions in sufficient detail to develop, test, and validate predictive models of chemical reaction rates. Predicted and measured reaction rates will be used in computer models for the design of new combustion devices with maximum energy efficiency and minimum, undesired environmental consequences.

The research supported by the chemical physics program for the molecular characterization of chemical dynamics at surfaces is aimed at developing predictive theories for surface-mediated chemistry such as is encountered in industrial catalysis or environmental processes. Surface-mediated catalysis reduces the energy demands of industrial chemical processes by bypassing energy barriers to chemical reaction. Surface-mediated catalysis is used to remove pollutants from combustion emissions. At the molecular level, surface-mediated catalysis is not well understood. New catalysts are few; improvements come principally from modification of known catalytic materials. There is no body of organized knowledge such as exists for the field of organic chemistry that may be used to find new catalysts for novel or existing processes. The knowledge gained from this research program will guide in the development of a predictive capability for surface chemistry.

Scientific Challenges:

- Improve and expand experimental measurement of key reaction rates of transient species at elevated temperatures.
- Develop spectroscopic probes of highly energetic, unstable molecules in complex reacting and radiating mixtures.
- Develop computational approaches of acceptable precision for the calculation of potential energy surfaces for ground and excited electronic states and their conical intersections for chemically important species including free radicals.
- Improve scaling with number of atoms to facilitate computations on large molecules.

- Improve methods for calculating chemical reaction rates from detailed chemical dynamics, including reactions without barriers for which statistical theories do not apply.
- Develop improved multiscale methods for dealing with systems exhibiting many orders of magnitude differences in spatial and temporal scales such as those found in turbulent combustion.
- Improve the time-to-impact of fundamental insights in chemical physics on next-generation devices and processes.
- Develop and apply new experimental methods for characterizing site structure and reaction mechanisms at interfaces.
- Characterize high-energy electron- and photon-stimulated processes at environmental interfaces.
- Design quantitative models for condensed-phase solvation that include polarization and charge-transfer effects.
- Develop new theoretical time-domain and frequency-domain simulation tools for computing structural, transport, and optical properties of nanoscale systems.

Funding Summary:

Dollars in Thousands

	FY 2005	FY 2006	FY 2007 Request
Chemical Physics Research	32,946	31,866	37,813
Combustion Research Facility	6,437	6,251	6,805
Chemical Physics Research (Total)	39,383	38,117	44,618

These funds provide support for about 130 principal investigators along with their graduate students and postdoctoral associates. Programs at the laboratories are multi-investigator efforts on problems that require extensive participation by senior scientists and postdoctoral associates.

Performer	Funding Percentage
DOE Laboratories	72 %
Universities	27 %
Other	1 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

The focus of the chemical physics program is the development of a molecular-level understanding of gas-phase, condensed-phase, and interfacial chemical reactivity of importance to combustion, catalysis, and environmental preservation. The desired predictive capability spans the microscopic to macroscopic domains–required is the ability to compute the results of individual molecular interactions as well as their complex, collective behavior in real-world devices. Currently, an increased emphasis is on theories and computational approaches for the structure, dynamics, and kinetics of open shell systems and on the interaction of chemistry with fluid dynamics. In surface chemistry, continued emphasize is on the development of a structural basis for gas/surface interactions, encouraging site-specific studies that measure local behavior at defined sites. At interfaces, emphasize is on aqueous systems and the role of solvents in mediating solute reactivity. Expanding into the future, plans are to enhance the use of computer-generated mechanisms and models in combustion science; initiate efforts that examine the reactivity of heteroatom-containing molecular building blocks of coal; and probe the chemical physics of energy transfer in large molecules, the molecular origins of condensed phase behavior, and the nature and effects of non-covalent interactions including hydrogen bonding. These molecular phenomena impact numerous DOE and national needs.

Research Activity: Photochemistry and Radiation Research

Division:	Chemical Sciences, Geosciences, and Biosciences
Primary Contact:	Mary E. Gress (mary.gress@science.doe.gov; 301-903-5827)
Team Leader:	Eric A. Rohlfing
Division Director:	Eric A. Rohlfing (Acting)

Portfolio Description:

This activity supports photochemical studies relevant to capture and conversion of solar energy, and fundamental studies in radiation chemistry. The solar photochemistry research encompasses physical chemical aspects of natural photosynthesis, charge separation by donor-acceptor models and nanoscale inorganic/organic assemblies, photocatalytic fuel-forming reactions, photoelectrolysis of water for solar hydrogen production, and photoelectrochemistry. Bioinspired photosynthetic models seek to mimic the key aspects of photosynthesis: the antenna, reaction center, catalytic cycles, and product separation. Research in radiation chemistry investigates fundamental chemical effects produced by the absorption of energy from ionizing radiation. Highly reactive transient intermediates, and the kinetics and mechanisms of their chemical reactions, are explored in the liquid phase and at liquid/solid interfaces. Research is supported on heavy ion radiolysis, models for track structure and radiation damage, free radical reactions in supercritical fluids, and radiolytic reactions in ionic liquids. Specialized accelerator facilities for electron pulse radiolysis are supported at Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), and the Notre Dame Radiation Laboratory. A novel Terawatt Ultrafast High Field Facility under development at ANL will offer capability for ultrafast electron-pulse radiolysis.

Solar photochemical energy conversion is an important long-range option for meeting future energy needs. Increasing worldwide demands for energy will need to be met with technologies such as solar photoconversion that do not produce greenhouse gases. An attractive alternative to semiconductor photovoltaic cells, solar photochemical and photoelectrochemical conversion processes produce fuels, chemicals, and electricity with minimal environmental impact and with closed renewable energy cycles. Artificial photosynthesis can be coupled to chemical reactions for generation of fuels such as hydrogen, methane, or complex hydrocarbons. The work in this activity is complementary to and coordinated with studies of natural photosynthesis within the BES activity Molecular Mechanisms of Natural Solar Conversion. A strong interface with the Office of Energy Efficiency and Renewable Energy (EERE) solar energy technology programs exists at the National Renewable Energy Laboratory (NREL), involving shared research, analytical, and fabrication facilities. Fundamental studies of radiation chemistry are of importance in understanding chemical reactions that occur in radiation fields of nuclear reactors, including in their fuel and coolants, and in the processing, storage, and remediation of nuclear waste. Such understanding is required for effective nuclear waste remediation and for design of next-generation nuclear reactors that might employ special media, such as supercritical fluids as coolants. The radiation chemistry of ionic liquids is relevant to their use as fuel-cycle separation solvents. The fundamental research in this activity coordinates with that performed in the BES Chemical Physics activity and is relevant to the Office of Nuclear Energy, Science and Technology (NE). Radiation-induced chemistry is also of importance in biological damage from nuclear weapons, from natural radiation sources, and in therapeutic uses of radiation.

Unique Aspects:

This activity is the dominant supporter (85%) of solar photochemistry in the United States and the sole supporter of radiation chemistry. Specialized electron pulse radiolysis facilities at Notre Dame, ANL, and BNL serve the academic research community, industrial users, and other Department of Energy (DOE) national laboratories. A laser-driven electron accelerator at BNL features a 10 picosecond pulse width and the capability for synchronized electron pulse-laser pump-laser probe experiments.

Relationship to Other Programs:

The solar photochemistry research effort interfaces with activities in BES, including: Energy Biosciences activities in biochemical aspects of photosynthesis; Chemical Physics theoretical calculations of excited states and computational modeling; Catalysis and Chemical Transformations investigations of electron transfer reactions in homogeneous and microheterogeneous solutions, and advanced catalytic materials; and the Materials Sciences and Engineering Division efforts in fundamental photovoltaics research. The research is relevant to EERE activities in the Solar Energy Technologies Program on photovoltaics and in the Hydrogen, Fuel Cells and Infrastructure Technologies Program on hydrogen production.

The radiation sciences activity interfaces in BES with Catalysis and Chemical Transformations in reaction kinetics in homogeneous solutions and Mechanical Behavior of Materials and Radiation Effects in radiolytic damage to glasses and radiation-induced corrosion of structural materials. There are also important interfaces with NE activities on nuclear reactors, and nuclear waste processing and storage. Radiolytic processes in solution, particularly heavy ion radiolysis, are of interest to the National Institutes of Health (NIH) regarding radiation damage to biological systems in medical diagnosis and therapy.

Significant Accomplishments:

Stratospheric ozone depletion by chlorofluorocarbons was predicted by F. Sherwood Rowland of UC, Irvine, in 1974. Professor Rowland’s research, solely supported by this activity, involved the chemistry of “hot” chlorine atoms produced by nuclear recoil and complementary photolytic reactions. Rowland was awarded the Nobel Prize in 1995. Radiotracers for nuclear medicine were pioneered by Alfred Wolf at BNL. The “special pair” model for electron donor chlorophyll molecules in photosynthesis was introduced by Joseph Katz and James Norris of ANL. Photosynthetic molecular models for light to chemical energy conversion were developed by Michael Wasielewski of ANL and by Professors Gust, Moore, and Moore of Arizona State University. The “inverted region” in Marcus electron transfer theory was verified in pulse radiolysis experiments by John Miller at ANL.

Mission Relevance:

Solar photochemical energy conversion is a long-range option for meeting the world’s future energy needs. An alternative to solid-state semiconductor photovoltaic cells, the attraction of solar photochemical and photoelectrochemical conversion is that fuels, chemicals, and electricity may be produced with minimal environmental pollution and with closed renewable energy cycles. A strong interface with EERE solar conversion programs exists at NREL, involving shared research, analytical and fabrication facilities.

Radiation chemistry methods are of importance in solving problems in environmental waste management and remediation, nuclear energy production, and medical diagnosis and radiation therapy.

Scientific Challenges:

In solar photoconversion, knowledge gained in charge separation and long-distance electron transfer needs to be applied in a meaningful way to activation of small molecules (CO_2, N_2, and H_2O) via photocatalytic cycles. The major scientific challenge for photoelectrochemical energy conversion is that small band gap semiconductors capable of absorbing solar photons are susceptible to oxidative degradation, whereas wide band gap semiconductors, which are resistant to oxidative degradation in aqueous media, absorb too little of the solar spectrum. Ongoing research activities include multibandgap, multilayer cascade-type semiconductors, photosensitized nanoparticles, and surface coatings that protect against photocorrosion. Experimental and theoretical studies on photosynthetic pigment-protein antenna complexes should lead to advances in design of efficient and robust artificial light-collecting molecular assemblies. Computational chemistry methods incorporating recent advances in calculation of excited states should be developed and applied in design of photocatalysts and molecular dynamics simulations in artificial photosynthesis. Fundamental studies on photochemical reaction pathways offer opportunities for less energy intensive and more environmentally benign processing of specialty chemicals and high volume industrial intermediates.

A recent workshop “Research Needs and Opportunities in Radiation Chemistry” identified new directions, connections, and impacts of radiation chemistry. A common theme is the need to explore radiolytic processes that occur across solid-liquid and solid-gas interfaces, where surface chemistry can be activated and changed by radiolysis. Solid-liquid interfaces abound in nuclear reactors and high level radioactive wastes. Colloidal particles participate in gas production, gas retention, and in organic degradation of high level wastes. In regard to environmental remediation, radiation chemistry is one of the most promising advanced oxidation processes for degradation of organic pollutants. A more fundamental understanding of radiolytic reactions in heterogeneous media is needed in order to predict and control radiation chemical transformations in complex environmental systems. A subpicosecond electron accelerator under development at ANL will enable investigation of the primary events in radiation chemistry, now virtually unknown except for theoretical models, wherein fundamental processes link physics to the chemistry of radiolysis.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
30,446	25,489	32,007

Performer	Funding Percentage
DOE Laboratories	67 %
Universities	33 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

The program provides funding for 53 university grants supporting about 53 graduate students, 50 postdoctoral research associates, and partially supporting about 59 faculty. There are nine programs at DOE national laboratories supporting 45 senior staff and 46 graduate students and postdoctoral research associates. Programs at the laboratories are multi-investigator efforts on problems that require extensive participation by senior scientists and postdoctoral associates. In photochemistry, major research groups are supported in inorganic photochemistry and electron transfer at BNL; in photoelectrochemistry at NREL, Notre Dame, and Pacific Northwest National Laboratory (PNNL); and in photosynthesis at ANL and Lawrence Berkeley National Laboratory (LBNL). Many of the research efforts at the national laboratories involve strong collaborative interfaces with university and industrial communities. The radiation chemistry effort is centered at specialized electron pulse radiolysis facilities at Notre Dame, ANL, and BNL. The Notre Dame Radiation Laboratory serves as the primary radiation research user facility, hosting approximately 40 users/year from academia and industry.

Projected Evolution:

In solar photochemistry, an increased emphasis on solar water splitting will explore new semiconductor, molecular, and hybrid systems for photoconversion. Modern combinatorial techniques will broaden and accelerate the search for new semiconductor and molecular structures. Novel quantum size structures, such as hybrid semiconductor/carbon nanotube assemblies, fullerene-based linear and branched molecular arrays, and semiconductor/metal nanocomposites, will be examined that will allow for more complete use of the solar energy spectrum. Unresolved basic science issues in photocatalysis will be explored in coupling photoinduced charge separation to multielectron, energetically uphill redox reactions. Photoconversion systems will be investigated that are based on organic semiconductors and conducting polymers, which are inexpensive and easy to manufacture. An enhanced theory and modeling effort is needed for rational design of artificial solar conversion systems. Of particular interest is the calculation of factors controlling photoinduced long-range electron transfer, charge injection at the semiconductor/electrolyte interface, and photoconversion in biomimetic assemblies for solar photocatalytic water splitting.

Electron pulse radiolysis methods will investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Radical ion excited states will be studied in novel synchronized electron pulse-laser pump-laser probe experiments. Fundamental studies on reactivity of nitrogen oxides in aqueous solution are pertinent to understanding radiolytic degradation of nuclear tank waste. Studies of solvent effects on free radical reaction rates in supercritical fluids are relevant to next-generation supercritical water-cooled nuclear power plants. Subpicosecond electron pulse radiolysis is being developed at ANL based on a table top terawatt laser system. Electron pulses are produced by focusing terawatt laser pulses into a supersonic helium gas jet. The approach is different from the laser-driven photocathode method employed at pulse radiolysis facilities at BNL, Osaka, and Paris where the time resolution is 7 ps, 0.2 ps, and 2 ps, respectively. Electron pulse radiolysis studies on the previously unexplored femtosecond time scale are proposed on solvation and thermalization of electrons in water; the dynamics of solvation and prethermalized species; solvation in confined media such as mesoporous silica and micelles; and charge injection into metal oxides. In the more distant future, the ability with the terawatt ultrafast high field facility to generate simultaneously subpicosecond electrons and x-rays will be exploited for detection of structural changes upon electron injection.

Research Activity:	**Energy Biosciences Research**
Division:	Chemical Sciences, Geosciences, and Biosciences
Primary Contact(s):	Richard V. Greene (Richard.Greene@science.doe.gov; 301-903-6190)
Team Leader:	John C. Miller (Acting)
Division Director:	Eric A. Rohlfing (Acting)

Portfolio Description:

This activity supports fundamental research required to understand and use biological energy, and to adapt strategies used by plants and microorganisms to capture, store, and mobilize energy. The program relies upon biochemical, physiological, and genetic methods to investigate and manipulate organisms and their biological processes. Emphasis is given to areas where these biological sciences intersect with energy-relevant chemical sciences; these include: (1) Mechanistic, molecular and biophysical studies on photosynthetic energy capture by plants and microbes. This entails research on light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide and initial reactions of carbon fixation and carbon storage. (2) Regulation of plant growth and development. Projects supported in this area focus on mechanisms that generate differentiated cells and cell-type determinations that are central to changing the properties and/or relative amounts of plant tissues for future use. (3) Understanding and manipulating plant biochemistry to increase levels of desirable components. This thrust investigates plant components with state-of-the-art biophysical, biochemical and chemical approaches, as well as ways in which plants generate and assemble components using the tools of biochemistry, physiology, and structural biology. (4) Metabolic pathways. Projects in this area examine biological syntheses and molecular interconversions with emphasis on novel systems for material production and chemical catalysis. (5) *In-situ* imaging of biological energy-tranduction systems. This research provides fundamental structural, chemical and biophysical knowledge required to improve natural light-harvesting and energy transformation systems, as well as for the design of biomimetic solar conversion systems. (6) Non-covalent biological interactions. Projects focus on mechanisms that govern self-assembly of biological components into complex systems, as well as studies that allow for their self repair. (7) Partitioning in plants and microbes. Priority is placed on projects that will allow for intelligent design of bioseparations and bioinspired separation technology.

Unique Aspects:

The Energy Biosciences program is the sole federal program devoted to fundamental science that underlies the use of biological systems to produce and conserve energy. It occupies an essential niche within the Department of Energy (DOE) at the interface between the life sciences and physical sciences and, thereby, promotes multi- and cross-disciplinary research activities. The program will generate a science base to inspire future energy-related biotechnologies and technologies that mimic biological systems.

Relationship to Other Programs:

The research effort interfaces with several activities within BES, including Photochemistry and Radiation Research in the area of biomimetic photosynthetic systems and Catalysis and Chemical Transformations in the area of biocatalysis. The program also supports basic research that may influence the directions of biotechnology-related programs in the DOE Office of Biological and Environmental Research, the Office of Energy Efficiency and Renewable Energy, the Office of Fossil Energy, and the Office of Environmental Management. The program collaborates and coordinates its activities with the National Science Foundation, U. S. Department of Agriculture, and National Institutes of Health in areas of mutual interest where there are multiple benefits.

Significant Accomplishments:

The program has a rich history of scientific impact. Among longer term accomplishments are the determination of the biosynthetic pathway for methane production from CO_2 and molecular hydrogen, the elucidation of the biochemistry and genetic regulation of plant lipid synthesis, determining the carbohydrate chemistry and structure of plant cell walls, and providing a central role in developing *Arabidopsis thaliana* as a model plant experimental system. Scientists supported by the program have received numerous awards and prizes including the 1997 Nobel Prize to Dr. Paul Boyer for his work on ATP, the energy currency of living systems.

Mission Relevance:

Enhanced understanding regarding how plants and microbes as biological systems capture solar energy through photosynthesis, biochemically transduce it, and store photosynthetically-fixed carbon into a variety of organic compounds is essential for future energy independence. The program strives for mechanistic knowledge that will provide potential technical options to use whole plants and microbes, their components, or biomimetic systems in energy-related processes. New commercial activities in ethanol production, pulp and paper manufacturing, and *in planta* production of oils are examples of technical options built on the foundations laid by the Energy Biosciences program.

Scientific Challenges:

Traditionally, mechanistic biology has been summarized and catalogued in relatively simple linear models. Analysis of both spatial and time-dependent dynamics and its subsequent integration in a coherent fashion represents a significant challenge, but also new opportunities. This is relevant to much needed molecular and biophysical studies on real-time control of photosynthesis, particularly mechanisms of light harvesting and energy transduction in microbes and chloroplasts as well as maintenance of the biological integrity of these systems. Understanding biological interactions that occur on the nanoscale is an immense challenge as well, but, when coupled to advances in molecular biology, it offers considerable dividend. An enormous scientific challenge facing all biology is to assimilate the vast amounts of genomic-sequence data and associate them with specific biochemical, physiological, and developmental processes. Studies specific to energy-related organisms and their life processes must be rationally integrated with the broader, interdisciplinary efforts, such as with the chemical and physical sciences.

Funding Summary:

Dollars in Thousands

	FY 2005	FY 2006	FY 2007 Request
Molecular Mechanisms	13,640	12,411	18,188
Metabolic Regulation of Energy Production	19,427	17,554	17,601
Energy Biosciences Research (Total)	33,067	29,965	35,789

Performer	Funding Percentage
DOE Laboratories	9 %
Universities	90 %
Other	1 %

Funding numbers do not include awards for conferences or training activities.

Projected Evolution:

Plant sciences research supported at DOE has evolved considerably from the late 1940s, when the emphasis was on radiation damage and breeding to demonstrate the peaceful use of the atom. Recent advances in sequencing plant genomes provide new opportunities to leverage the traditional strengths of the program in genomics and biochemistry with powerful capabilities in imaging and computation. For example, this will allow for an unprecedented biophysical understanding of photosynthesis at the nanoscale. Similarly, molecular and biochemical studies on microbes with novel metabolic capabilities, tolerance of extreme conditions, and/or efficient catalytic mechanisms will allow for efficient energy and chemical conversion strategies. Through an integrated approach, efficient future conversions can likely be accomplished by a plant in conjunction with a microorganism (the coupling of green and white biotechnology).

A unique aspect of biological systems is their ability to self-assemble and self-repair. These capabilities occur via complex, poorly understood processes, and much work is needed before application to synthetic or semi-synthetic energy systems may be realized; however, the potential in this area of prospective study is immense. Future impact is also envisioned through increased research in natural photosynthesis to serve as a basis for biomimetic solar conversion systems, amplified use of experimental and computational tools from the physical sciences (ultrafast laser spectroscopy, current and future x-ray light sources, quantum chemistry) to probe biological energy transduction systems, and enhanced efforts in molecular biology and biochemistry that are relevant to improved chemical processes.

Research Activity: Catalysis and Chemical Transformations

Division: Chemical Sciences, Geosciences, and Biosciences
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Team Leader: John C. Miller
Division Director: Eric Rohlfing (Acting)

Portfolio Description:

This activity supports basic molecular-level research to understand chemical catalysis and electrocatalysis, and to develop principles and predictive methods for the rational design of catalysts. It encompasses all types of catalysts for organic and inorganic synthesis and transformation reactions, including organometallic complexes, hybrid organic-inorganic compounds or porous solids, bio-inspired catalysts, interfaces of metals, semiconductors and non-metallic compounds such as oxides, carbides, and nitrides. Special emphasis is placed on nanocatalysis, to understand and use the enhanced catalytic properties that emerge at the nanoscale. Its research portfolio addresses catalytic model systems of relevance to fossil and renewable energy production, storage, and use; environmental remediation; materials synthesis; fuel cell reactions; and photocatalytic conversions. It promotes the use and the co-development of advanced synthetic, spectroscopic, and theoretical techniques that pertain to the intrinsic needs of catalysis research, such as complex but controllable compositions and structures and wide scales of time and space resolution. Nanoscale design, multiscale theory, modeling and simulation, and femtosecond and synchrotron-based spectroscopic techniques present unique opportunities for the acquisition of new knowledge in catalysis. This activity is the nation's major supporter of catalysis research as an integrated multidisciplinary activity, assembling a body of researchers from several branches of science.

Unique Aspects:

This activity funds the largest fraction of basic research in catalysis in the federal government. It seeks to cross the barriers between heterogeneous, homogeneous, and bio catalysis. The integration promotes synergism among disciplines and innovation in fundamental approaches as well as applications. In terms of instrumentation, this program has helped with the establishment of surface science and inorganic synthesis laboratories at universities and encourages the use of large-scale facilities at the Department of Energy (DOE) national laboratories. Principal investigators use synchrotron, neutron and electron sources and computational tools to significantly advance catalysis research.

Relationship to Other Programs:

This activity relates to other activities within BES. The Catalysis and the Chemical Physics activities have complementary goals in the areas of surface science, surface chemistry, and quantum mechanical theory, molecular modeling, and simulation of catalytic-related phenomena. The Catalysis and Photochemistry activities also complement one another in the support of fundamental photocatalysis and photoelectrocatalysis, which are relevant to solar photoconversion and photochemical synthesis. The Catalysis and Separations activities share their concern and in some instances co-support synthetic research for zeolitic, mesoporous, hybrid, and caged materials. The Catalysis and Heavy Elements Chemistry activities also share interest in the design and synthesis of ligands and coordination compounds of lanthanides. The BES synchrotron facilities have beamlines used by Catalysis researchers, in particular the National Synchrotron Light Source (NSLS), Advanced Photon Source (APS), Intense Pulsed Neutron Source (IPNS), and Advanced Light Source (ALS). The BES Nanoscale Science Research Centers (NSRCs), in particular the Center for Functional Nanomaterials (CFN) and the Center for Nanophase Materials Sciences (CNMS), also have thrust areas that address catalysis research, and hence share some of the Catalysis activity goals.

Within DOE, the activity of Catalysis produces research outcomes of relevance to programs of the Office of Energy Efficiency and Renewable Energy and the Office of Fossil Energy. These programs have collaborated during the review of proposals in relevant initiatives, such as the Hydrogen Fuel Initiative.

The activity is coordinated with other federal agencies. At the National Science Foundation (NSF), heterogeneous and bio catalysis are funded within its Engineering Directorate while homogeneous catalysis is funded within the Math and Physical Sciences Directorate (Organometallic and Inorganic Chemistry program). Also at the NSF, the surface science and materials aspects of catalysis are spread among three divisions (Chemistry, Materials, and

Chemical and Transport Systems). The National Institutes of Health (NIH) funds the health-related applications of homogeneous, enzymatic, and bio catalysis; the Environmental Protection Agency (EPA) funds the application of catalysis to environmental remediation; and the Office of Naval Research (ONR) and Army Research Office (ARO) support the application of catalysis to military purposes.

Significant Accomplishments:

The science and practice of catalysis over the last several decades have led to many achievements of fundamental interest. A significant contribution has been made to the current molecular-level understanding of catalytic cracking of hydrocarbons in zeolites, reforming of hydrocarbons over supported bimetallic alloys, and desulphurization of heteroaromatics over supported metal sulfides. Reactions of importance in environmental chemistry, such as removal of NO_x, have been studied in detail over model single crystal metals and supported metals. Results of those investigations have dramatically improved the knowledge of catalyst structure-reactivity relationships. This activity has also led to fundamental advances in the catalysts required for the selective oxidation of hydrocarbons for the manufacturing of monomers, fine chemicals, and fuel additives. During the past decade, one of the most significant accomplishments in homogeneous catalysis was the development of novel single-site metallocene catalysts for polymerization of alkenes. The control of polymer tacticity resulted in property enhancement and a largely expanded use of polyalkene plastics, from extending the shelf life of food we buy to enhancing the efficiency of the cars we drive. Other very significant achievements were the catalytic synthesis of organic acids by alcohol carbonylation and the generation of important monomers by olefin metathesis. More recently, the selective oxidation of C-H bonds was achieved both homogeneously and heterogeneously. For their achievements, researchers in this program have been widely honored by scientific societies, as they have received three-quarters of the awards in Organometallic Chemistry given by the American Chemical Society, all but one of the fundamental catalysis awards given to U.S. academics by the North American Catalysis Society, And several international awards, including the Nobel Prize in Chemistry for 2006.

Mission Relevance:

Catalytic transformations impact virtually all of the DOE energy missions. Catalysts are needed for all of the processes required to convert crude petroleum and natural gas into clean burning fuels. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added chemicals. Catalytic science has impacted the technology used to clean up environmental pollutants, such as unwanted products from chemical production or from combustion, or by transforming toxic chemicals into benign ones, such as chlorofluorocarbons into environmentally acceptable refrigerants.

Scientific Challenges:

The grand challenge for this area of research is the *a priori* molecular-level design and synthesis of catalysts with controlled reactivity and durability. Such knowledge is of relevance for the production of catalysts that convert natural resources into energy or desired products in an energetically efficient and environmentally benign manner. That challenge can be met by coordinating fundamental research on chemical synthesis, structural characterization, mechanistic studies, and theoretical interpretation.

The current challenge in inorganic synthesis is the atomistic and molecular control of structure, shape, and functionality, all of which can be facilitated by the development of libraries of modular ligands. For the particular case of biomimetic catalyst development, synthesis and use of versatile ligands must be promoted. Likewise, air- and water-resistant complexes must receive priority. The control of macromolecular structure continues to be a challenge. Secondary structures that produce shape-selective reaction environments must be attained by the use of, for example, dendrimers, polypeptides, zeolites, and imprinted media.

In solid state synthesis, the current frontier is to produce catalytic materials with nanoscale control of composition, homogeneity, shape, and structure. A challenge is to design molecular precursors and convert them into solid-state structures with desired chemical functionalities that are durable under reaction conditions. Traditional routes of surface chemistry, aqueous-solution chemistry, and high-temperature chemistry need to be complemented by softer routes. For example, coordination chemistry may be used to build nanoparticles that are surface-functionalized with metal compounds. Organic or biological strategies may then be used to arrange the particles into preconceived patterns. These arrangements will provide molecular recognition properties (for example, size, shape, chirality, and hydrophobicity).

The characterization of synthetic catalysts demands higher spatial and time resolution under *ex situ* and *in situ* conditions. Both electronic and atomic structures must be correlated with secondary and macrostructure and their time-resolved evolution. The kinetically significant intermediates must be identified and discriminated from those species or moieties that contribute to selectivity and from those that are merely inactive. This is a particularly crucial need in solid-mediated catalysis and biocatalysis.

The study of reaction mechanisms will be promoted by the synergistic use of theory, simulation, and experimentation. In particular, identification and structural characterization of the transition states still remains a challenge for most reactions. Classical labeling, trapping and molecular probe experiments must be complemented with time-resolved *in-situ* spectroscopy in order to acquire information on bonding dynamics. The development of chemo-, regio-, and stereo-selective reactions is of primary importance to the advancement of the science of catalysis, since those reactions present the highest demands on catalysts. Conformers at equilibrium are usually separated by barriers of less than 3 kcal/mol. While high selectivity has been obtained with homogeneous catalysts in selected instances, heterogeneous catalysts require substantially more study, possibly with help from biomimetics.

Catalysis of bond cleavage and reformation has, for the most part, been restricted to hydrocarbons (CC, CH bonds), halogenated compounds (CX bonds), and nitrogen and sulfur containing compounds (CS, CN bonds). Moreover, past and current research has also addressed the selective addition of oxygen, hydroxyl, or nitrogen to hydrocarbon and aromatics. For homogeneous catalysis, the challenge is to carry out these selective reactions under solvent-less conditions or with green solvents such as supercritical CO_2, while maintaining stability. For heterogeneous catalysis, the challenge is to work at low temperature and pressure conditions with high activity and selectivity. For both types of catalysis, a major challenge is to obtain selective conversion for reactants such as short-chain saturated hydrocarbons and other refractory molecules. Likewise, new challenges for all types of catalysts have arisen in activating molecules and materials derived from biorenewable resources.

Besides hydrocarbon chemistry, other challenges reside in the elucidation of the catalytic mechanisms for the synthesis of molecular and nanomaterials. For example, in the catalytic synthesis of carbon nanotubes, chirality control has remained elusive because of lack of understanding of the structure-determining steps. As another example, the nucleation and subsequent growth of silicon nanowires from silane or its derivatives on molten gold nanoparticles proceed through catalytic pathways that must be understood. Finally, the synthesis of compound semiconductors and more complex nanomaterials constitute an excellent challenge for the development of catalytic science and its application to a new area.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
37,871	38,107	47,459

Performer	Funding Percentage
DOE Laboratories	58 %
Universities	38 %
Other	4 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

The laboratory programs are multi-investigator efforts and make use of specialized facilities at Lawrence Berkeley National Laboratory, Brookhaven National Laboratory, Oak Ridge National Laboratory, Argonne National Laboratory, and Ames Laboratory, usually involving collaborators from universities.

Projected Evolution:

The science of catalytic chemistry is still emerging. A wealth of experimental information has been accumulated relating catalytic structure, activity, selectivity, and reaction mechanisms. However, for phenomenological catalysis to evolve into predictive catalysis, the principles connecting those kinetic phenomena must be more clearly and thoroughly identified.

Better understanding of the reactivity of matter will result from more complete integration of experiment and theory, reproducible synthesis of catalysts, and thorough characterization of catalysts and reactions. An effort is needed to promote scientific cooperation among groups with complementary expertise in synthesis, structural characterization, intermediate and transition state characterization, dynamics simulation, and kinetics determination. National laboratories or university centers may serve as focal points for knowledge integration.

Following from the specific scientific challenges outlined above, it has become apparent that the convergence of heterogeneous, homogeneous, and biocatalysis must be promoted. Ideas and approaches motivated by biological reaction systems will be used to derive new biomimetic homo- or heterogeneous analogues. For example, two such particular ideas are the use of long-range or secondary structure to affect not just selectivity but also activity of inorganic catalysts, and the use of tunable structural flexibility to affect reaction pathways and hence selectivity.

New single investigator efforts are expected to be focused on the challenges mentioned. The following examples illustrate the areas where mechanistic understanding and new methodology are needed: (a) synthesis of hybrid organometallic-heterogeneous catalysts from molecular precursors such as organometallic or cluster compounds or organic-inorganic host-guest complexes; (b) synthesis of mixed metal inorganic compounds and derived high-temperature catalysts consisting of crystalline nanoporous structures with precisely positioned chemical functions; (c) selective functionalization of saturated hydrocarbons or stereoselective functionalization of complex molecules by heterogeneous catalysis; (d) characterization of kinetically relevant intermediates and catalyst dynamics with high spatial and time-resolution and *in situ* spectroscopy, microscopy and diffraction, and in particular, with synchrotron and neutron-based techniques and advanced computational techniques; (e) environmentally benign transformations using solvent-less homogeneous catalysis, low-temperature heterogeneous reactions, and tandem or programmable catalysis, i.e., precise matching of functionalities among dissimilar catalysts.

Research Activity: Separations and Analysis

Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact: William S. Millman (william.millman@science.doe.gov; 301-903-5805)
Team Leader: John C. Miller
Division Director: Eric Rohlfing (Acting)

Portfolio Description:

This activity addresses the scientific principles that underlie energy-relevant chemical separations and analytical methods, capitalizing on the relationships between these two areas of chemistry and Heavy Element Chemistry. It is focused around four main thrust areas along with a small assortment of other science themes. The thrust areas are:

- Laser based techniques: These rely on laser based spectroscopies and other techniques that provide the basis for analytical methods. Besides spectroscopy, lasers are used as probes or the initiator of a process that is ultimately quantified.
- Nanoscale science approaches to separations and analysis: These projects focus on aspects of the nanoscale that can be exploited to affect a separation or to understand the influence of the nanoscale on separations. These include nanoscale transport, synthesis of nanoscopic pores and structures, analysis of nanoscopic materials and relationship between nanoscale properties and chemical properties unique to the nanoscale.
- Ionization processes in analysis: This thrust is the major focus of mass spectrometry programs. It includes surface preparation and modification associated with mass analysis, and the interactions between ions and molecules and the transport and acceleration of ions in a vacuum and in the presence of various applied fields.
- Metal-adduct complexes for separations: This thrust is largely associated with extraction of trans-actinide elements. It includes the synthesis of ligands uniquely capable of interacting with specific elements. It also includes supramolecular complexes and other large structures such as micelles that can uniquely interact with transuranics along with their ability to attach or otherwise interact with surfaces and the resulting impact on selectivity.

The remaining activities are composed of a variety of projects such as those related to analysis of catalysts and catalytic phenomena, NMR analysis, droplet formation, solvation, a variety of synchrotron based analyses, and a growing new area in chemical imaging.

Unique Aspects:

This activity represents the nation’s most significant long-term investment in solvent extraction, ion exchange, and mass spectrometry. The supported research is characterized by a unique emphasis on underlying chemical and physical principles, as opposed to the development of methods and processes for specific applications.

The portfolio for separations science emphasizes, but is not limited to, the separations of radionuclides and other metal ions, and seeks molecular-level understanding to support advances in both large-scale and analytical-scale separations. Molecular-level understanding is also sought for separations methods that have the potential to significantly impact energy use, such as membrane-based processes. Ionic liquids and supercritical fluid solvents are being explored with potential benefit to “green chemistry.” The use and impact of nanoscale and supramolecular structures on various separations processes are of growing interest.

The analytical research portfolio has historically emphasized mass spectrometry and seeks to elucidate the chemical and physical principles that underlie ionization and excitation processes and modern approaches to mass discrimination. A more recent sector of the portfolio seeks to understand and use the interaction of electromagnetic radiation with matter in phenomena such as molecular fluorescence, laser ablation and surface-enhanced Raman scattering. Hyphenated laser-mass spectrometry techniques such as MALDI-MS, laser ablation ICP-MS, and laser ionization ion mobility-MS are being explored. The extension of these ultrasensitive techniques to single-molecule detection and observation is being explored. Research to understand chromatography at the molecular level reflects the synergy between separations and analytical sciences. This activity also contributes to the maintenance of the scientific infrastructure required to meet as-yet-undefined challenges in separations and analysis.

Relationship to Other Programs:

The activity is closely coupled to the Department of Energy (DOE) stewardship responsibility for actinide and fission product chemistry and to its clean-up mission. The activity emphasizes the separations and analysis of actinide and fission product elements and their decay products. Some overlap and coordination with the BES Heavy Element Chemistry Program is natural. Similarly, elements of the analysis science portfolio benefit from cooperation with the BES Catalysis and Chemical Transformations, Chemical Physics, Materials Chemistry, and Atomic and Molecular Science Programs. The basic nature of the research has led to advances in technologies ranging from those that support nuclear non-proliferation efforts, to efforts in the President's Hydrogen Fuel Initiative, and to aspects of the Human Genome Project.

Significant Accomplishments:

This activity is responsible for such notable contributions as the concept of host-guest complexation, for which Professor Donald Cram (University of California, Los Angeles) shared the 1987 Nobel Prize in Chemistry; the use of the inductively coupled plasma (ICP) for emission and mass spectrometry; the development of the TRUEX process based on the ligand design work of Dr. Phillip Horowitz; Dave Dahl's development of SIMION, a program to simulate the motion of ions in fields that has become the standard tool internationally for development of ion lens; and, more recently, the development of BOB, a calixerene ligand that complexes Cs+ which is based on design and development work of Bruce Moyer at Oak Ridge National Laboratory (ORNL) and is being used to clean up waste tanks at Savannah River National Laboratory (SRNL).

Mission Relevance:

The success of the Manhattan Project was, in large part, due to our ability to develop industrial-scale processes for separating plutonium from irradiated fuel. Thus began the intense interest of DOE and its predecessor agencies in the science that underlies separations processes. The missions of DOE have evolved, and it must now face the legacy of accumulated wastes from the cold war era. Knowledge of molecular-level processes is required to characterize and treat these extremely complex mixtures and to understand and predict the fate of associated contaminants in the environment. In addition, separations science and technology have huge economic and energy impacts. For example, distillation processes in the petroleum, chemical, and natural gas industries annually consume the equivalent of 315 million barrels of oil (~5.4% of total petroleum consumption). It is further estimated that separations processes account for more than 5% of total national energy consumption. Separations are essential to nearly all operations in the processing industries and are necessary for many analytical procedures.

Likewise, DOE and its predecessors were also driven to develop analytical methodologies to support their early missions. Nuclear and radiochemical analyses were supported and refined by developments in analytical separations, such as solvent extraction and ion exchange. A need for reliable potentiometric titration prompted the first use of operational amplifiers in analytical chemistry and led to a revolution in electrochemistry. Mass separations was required for assay in the form of mass spectrometry and, in the form of the calutron, served as the first method for the production of macroscopic quantities of separated isotopes of uranium and other elements. As with separations science, improved understanding of the underlying science is required to meet the analytical challenges presented by the legacy of the Cold War and the future challenges of DOE as its missions and responsibilities continue to evolve.

Scientific Challenges:

Challenges in separations science include the development of a deeper understanding of processes driven by small energy differences. These include self-assembly and molecular recognition, crystallization, dispersion, coalescence, and hysteresis in transport properties of glassy polymer membranes. The development of fundamental principles to guide ligand design for atomic and isotopic specific recognition and separations is also required. These, in turn, pose challenges to analysts to generate the understanding required to characterize amorphous materials through analysis of scattering data or other methods. Other analytical challenges include single-molecule detection and direct observation of bimolecular interactions and reactions. A deeper understanding of laser-material interactions as well as ionization and excitation sources for optical and mass spectrometric analyses is also required. Significant challenges are posed by elucidation of principles to underlie diagnostics at interfaces between synthetic materials and biomolecules, at oxide-aqueous interfaces, and to monitor spatial and temporal processes in, and on the surfaces of living cells. Though understanding at the molecular level is required, there is currently insufficient knowledge to extend that understanding from the molecular level to the nanoscale, to mesoscale, and finally, to macroscale phenomena. Pursuit of that knowledge presents a major challenge to this activity.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
15,490	17,287	24,041

Performer	Funding Percentage (2005)
DOE Laboratories	56%
Universities	44%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

This activity provides funding for about 50 university grants supporting, at any given time, on the order of 60-70 graduate students and 25-30 postdoctoral associates. In addition, 14 programs at DOE national laboratories support numerous senior staff, and additional students and postdoctoral associates. Programs at the national laboratories are typically multi-investigator efforts on problems that require extensive collaboration by senior scientists and postdoctoral associates. These programs act as the focal point for specific research efforts vital to the DOE mission. This activity supports research programs at ORNL, Argonne National Laboratory (ANL), and Pacific Northwest National Laboratory (PNNL), with smaller efforts at Ames Laboratory, and Lawrence Berkeley National Laboratory (LBNL). Many of the research efforts at the national laboratories involve collaborations with the university and industrial communities.

Projected Evolution:

Separations research will continue to advance the understanding of multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous materials and control of interface properties at the nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; solvation in supercritical fluids; field-enhanced mixing; and drop formation.

Analytical research will pursue the elucidation of ionization and excitation mechanisms for optical and mass spectrometry; single molecule detection, characterization, and observation; nano- and molecular-scale analytical methods; laser-based methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry; characterization of interfacial phenomena, with emphasis on chromatography; surface-enhanced Raman spectroscopy; and use of quadrupole ion traps to study gas-phase ion chemistry.

An expanded activity would support work to understand the underlying science needed to image molecular assemblies and molecules in space and time to enable new advances in science. The program is now in a position to begin doing experiments similar to those in microscopy that brought about a revolution our understanding of cells as the underlying structure that supports life.

Research Activity:	**Heavy Element Chemistry**
Division:	Chemical Sciences, Geosciences, and Biosciences
Primary Contact:	Lester R. Morss (lester.morss@science.doe.gov; 301-903-9311)
Team Leader:	John C. Miller
Division Director:	Eric Rohlfing (Acting)

Portfolio Description:

This activity supports research in the chemistry of actinide elements (a family of radioactive elements that includes uranium and plutonium), transactinides, and long-lived radioactive nuclear reactor fission products such as technetium. Areas of interest are the chemical bonding and reactivity of actinide ions in solids, solutions, and gases; synthesis, structure, and other properties of actinide materials; theoretical methods to predict heavy element electronic and molecular structure and reactivity; and chemical properties of the transactinide elements. The central theme is the unique chemical properties due to the electron orbitals available to and occupied by these elements, especially the 5f orbital.

The Heavy Element Chemistry program has determined the chemical properties of the transuranium elements since its genesis in the Manhattan Project. The present emphasis is the chemistry of technetium, uranium, neptunium, plutonium, and americium, driven by the necessity to characterize and control long-lived radioisotopes found at Department of Energy (DOE) legacy waste sites. Knowledge of the molecular speciation of stored actinide and fission products is necessary to predict the properties of these complex mixtures and to deal with them. This activity is coupled to the BES Separations and Analysis activity, to actinide and fission product chemistry efforts in the DOE Environmental Management Science Program, and to nuclear fuel cycle research of the DOE Office of Nuclear Energy, Science and Technology. This activity represents the nation's only funding for basic research on the chemical and physical principles governing actinide and fission product chemistry. The education of undergraduates, graduate students, and postdoctoral researchers at DOE national laboratories and universities is an important responsibility of this activity.

Unique Aspects:

This activity represents the only source of funding for basic research in the actinides and transactinides in the nation. Its major emphesis is to understand the underlying chemical and physical principles that determine their behavior. The activity is primarily based at national laboratories because of the special facilities needed in order to handle these radioactive materials safely.

Relationship to Other Programs:

This activity provides the fundamental understanding of the properties of the actinides, transactinides, and fission product elements that support DOE missions in advanced nuclear energy, stewardship responsibilities for defense programs, and environmental clean-up. The Heavy Element Chemistry program conducts unclassified basic research on all the actinide and transactinide elements, while applied programs generally limit their investigations to the chemical and material properties of specific elements and systems of strategic, economic, or programmatic interest. This activity also has close ties to the BES Separations and Analysis activity, which has a major focus on the separation of actinides and fission products from other elements.

Significant Accomplishments:

The Heavy Element Chemistry activity had its genesis in the Manhattan project. It continues today as the nation's only basic research program supporting the exploration of the physical and chemical properties of the transuranium elements. The early goal was to determine the chemical and physical properties of the new elements and to discover new elements. The chemical properties of the transuranium elements, especially plutonium, originally were determined from microscale experiments. The processes for the separation of plutonium from uranium and fission products on an industrial scale were developed and scaled up from these results. The inorganic chemistry of the elements through einsteinium (Es, atomic number 99) has been determined with small but weighable quantities of the elements. For the elements heavier than Es in the periodic table, tracer techniques and one-atom-at-a-time chemistry have been developed and carried out through element 108 to determine chemical properties. Organometallic chemistry has been enriched by discovery of many unique organoactinide compounds.

Taken together, the results from this activity have repeatedly confirmed the Seaborg hypothesis that the actinides are best represented in the periodic table as a 5f element series placed under the 4f (lanthanide) series. Interpretations of spectroscopic results have provided thermodynamic quantities such as oxidation-reduction potentials and enthalpies of sublimation. Specific electronic transitions determined in this activity have proven useful in developing processes for laser isotope separation of uranium and plutonium. Magnetic measurements have shown that the light actinide metals have delocalized 5f orbitals and resemble d-orbital transition metals, whereas the f electrons become localized at americium, element 95, so that the heavier actinide metals exhibit behavior similar to the rare earth metals.

Mission Relevance:

Knowledge of the chemistry of the actinide and fission product elements is necessary for the success of many of the DOE missions. In the area of nuclear energy, this activity provides the fundamental understanding of actinide and fission product chemistry that underpins the development of advanced nuclear fuels, as well as the predictions of how spent nuclear fuels degrade and radionuclides are transported under repository conditions. In the defense area, understanding the chemistry and material properties of specific actinides were key to the development of our nuclear deterrent, and now plays a major role in the stewardship of the nuclear stockpile. Driven by the necessity to identify and treat radioactive species in highly basic solutions found in many waste tanks at DOE sites, this activity has had a renewed emphasis on the molecular speciation of the lighter transuranium elements and fission products. Molecular speciation information is also needed to predict the fate of actinides and fission products accidentally released to the environment. Finally, the analytical chemistry methods developed under this activity have broad application across all the applied missions of DOE that deal with nuclear materials.

Scientific Challenges:

The role of the 5f electrons in bond formation remains the fundamental topic in actinide chemistry, providing the central focus for this program. The 5f orbitals participate in the band structure of materials that contain the light actinide metals and some of their alloys. Whether the 5f orbitals participate significantly in molecular compounds is still unclear. Molecular-level information on the geometry and energetics of bonding can now be obtained from experiments carried out at the Nation’s synchrotron light sources, and from multi-photon laser excitation studies. These new tools enable studies of actinides in the gas phase, as clusters, and at interfaces between solutions and mineral surfaces. Actinide and fission product samples must be handled with special consideration because of their radioactivity, which limits the types of experiments that can be safely conducted. For example, in the soft x-ray regime new sample preparation techniques need to be developed so that micro-quantities of well-characterized actinide samples can be measured using high vacuum techniques, or in "wet" cells to study liquid-solid interfaces.

Sophisticated quantum mechanical calculations that treat spin-orbit interactions accurately need further development so that they can be used for predicting the properties of molecules that contain actinides. Development and validation of such computer codes will provide a means for obtaining fundamental information about actinide species that are difficult to study experimentally, will predict the electronic spectra of important species, and will correlate the optical spectra with actinide molecular structure. Improved modeling of actinide transport requires understanding of the processes describing sorption on surfaces. Surface complexation models exist, but experimental validation of these models has not been readily available. Ultimately, experimentally validated theoretical calculations will be the key to understanding the role of the 5f electrons.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
10,506	9,354	17,128

Performer	Funding Percentage
DOE Laboratories	70%
Universities	20%
Other	10%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

This activity supports research in heavy element chemistry at universities, encouraging collaborations between university and DOE national laboratory projects in this area. Twenty-four undergraduate students, chosen competitively from universities and colleges throughout the United States, are taught actinide chemistry and radiochemistry each summer in two programs at Brookhaven National Laboratory (BNL) and San Jose State University. Graduate and postdoctoral students are educated to provide personnel for the technological challenges associated with the heavy elements.

Projected Evolution:

At the frontier of the periodic table, theoretical chemists predict the properties of actinides and transactinides in gaseous molecules, liquid clusters, and solid species using modern calculation tools such as density functional theory. Because most actinide species have partly filled 5f electron subshells and all have highly charged nuclei, both spin-orbit and relativistic effects must be included in the calculations. More sophisticated quantum mechanical calculations of actinide compounds and actinide species in environmental media are being developed. Heavy Element Chemistry theoretical research pursues advances in gas-phase chemistry that explore new reactivity patterns, photophysics, and photochemistry of actinide ions in their excited states, and in organoactinide chemistry.

Support of research to understand the chemical bonding of elements that have 5f electrons will lead to fundamental understanding of separations processes and to the design and synthesis of more effective preorganized chelating agents for the separations of particular actinide ions. Research in bonding, reactivity, and spectroscopic properties of molecules that contain heavy elements and of actinides in environmentally relevant species aids the development of ligands to sequester actinides in the environment and to remove toxic metals from the human body. Better characterization and modeling of the interactions of actinides with well-characterized liquid-solid interfaces, including mineral surfaces under environmentally relevant conditions, is needed.

Research on synthesis, crystal structure, and bonding in actinide solids leads to materials that are designed to be especially stable in environments such as nuclear fuels and nuclear waste forms. Spectroscopic investigations of new actinide materials and high-pressure studies of actinide metals elucidate the unique bonding properties and electronic characteristics attributable to 5f electrons. New facilities for safely handling radioactive materials at the synchrotron sources will permit more widespread use of techniques such as x-ray absorption spectroscopy and scattering on radioactive samples, providing detailed information on actinide speciation in crystalline and amorphous solids such as spent fuel and radioactive waste forms.

Research Activity: Geosciences Research

Division:	Chemical Sciences, Geosciences and Biosciences
Primary Contact:	Nicholas B. Woodward (Nick.Woodward@science.doe.gov; 301-903-4061)
Team Leader:	John C. Miller
Division Director:	Eric Rohlfing (Acting)

Portfolio Description:

This activity supports basic research in rock physics, analytical geochemistry, experimental and theoretical geochemistry, and flow and transport of subsurface fluids. The research seeks to understand how earth properties can be imaged and probed remotely at higher resolution than available with current technology or approaches. It develops analytical methodologies to probe ever smaller mineral domains to track complex reactive processes. It seeks understanding of the controls on complex multiphase reactions among solutions, particles, and surfaces at depth through new experimental methods and computational modeling and simulation of geologically significant processes. It seeks to understand the physics of fluid flow of complex reactive geofluids in highly heterogeneous porous and fractured media at depth. The research is designed to develop understanding of properties to enhance our ability to monitor, measure, and validate ongoing geological processes in the earth. It underlies our ability to track trajectories and rates of chemical and physical processes in the earth. It expands our understanding of the controls on critical geochemical and geophysical processes and provides the foundation for a predictive capability of the changes expected over time. New areas of interest include neutron research in the geosciences that will exploit the BES neutron scattering facilities and nanogeosciences research that challenges our understanding of how traditional measurement techniques of geological materials can accurately reflect geological processes and rates. Natural geosystems with wide ranges of length scales and time scales can be paradigms for how to test and model complex systems and emergent behavior in general.

Unique Aspects:

This activity has an agency-wide mandate to provide new knowledge as the foundation for targeted applications in energy and environmental quality. This activity is pioneering the application of x-ray and neutron scattering to geochemical and geophysical studies. It is the largest supporter of long-term basic research in shallow earth processes in the nation. The objective of this activity is to provide understanding sufficient for imaging, probing, and prediction of shallow earth processes, particularly those related to reactive flow and transport in fractured and porous geological media due to the importance of these problems to multiple Department of Energy (DOE) mission areas. It interacts collaboratively with research programs supported by the Offices of Biological and Environmental Research, Fossil Energy, Environmental Management, and Radioactive Waste Management through support for DOE national laboratory capabilities used by all of these offices. This research program provides enabling understanding for the DOE mission driven programs in environmental cleanup, geothermal energy development, higher-productivity hydrocarbon development, geological sequestration of CO_2 and other energy waste, and long-term monitoring and stewardship of DOE legacy sites. Unique strengths of the program lie in its emphasis on cutting-edge atomic-scale experimental, theoretical, and modeling studies in both geochemistry and geophysics built on the capabilities of national laboratory facilities and over a hundred university research projects.

Relationship to Other Programs:

The Geosciences Program provides 20% ($20M) of the nation's support for individual investigator-driven fundamental research (National Science Foundation (NSF) + DOE ~ $100M) in solid Earth sciences. BES focuses on a narrower range of fundamental issues than NSF (those critical to the DOE mission), particularly in shallow Earth environments, and exceeds NSF support in these areas. DOE user facilities in geosciences, particularly synchrotron x-ray beamlines, are available to all of the geosciences community within the United States.

Significant Accomplishments:

The GSECARS beamline has been built and commissioned (in collaboration with NSF-EAR) as a center for high-resolution analytical geochemistry for the whole Earth sciences community, including multiple DOE applied program users. Geoscience's participation in the BESSRC beamline brings those capabilities to the Earth sciences community as well. Geosciences research projects and a Geosciences workshop on Terrestrial Sequestration of CO_2 were the foundations for identifying research opportunities in this area for the Office of Science and the Office of Fossil Energy. Geosciences workshops have produced broadly applicable publications of Reactive Fluid Flow and Transport Modeling, and enhancing access to Geosciences user facilities which broadly circulate BES interests and approaches to these areas of importance for the DOE. Geosciences investigators have published major review volumes on Synchrotron Science related to Geosciences, Molecular Modeling applied to Geosciences, Nanophases in the Shallow Earth Environment, Biomineralization, Isotope Geochemistry, Biomineralization and Molecular Geomicrobiology .

Mission Relevance:

The activity contributes to the solution of Earth science-related problems in multiple DOE mission areas by providing a foundation of scientific understanding for applications such as (but not limited to): the potential of geophysical imaging of permeability; reactive fluid flow studies to understand contaminant remediation, or geothermal energy production; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance. The DOE applied activities focus on solutions to existing problems in the near-term (0-5 years) but seek fundamental research results as the foundation for their directed research and development efforts in the longer-term, both from the national laboratories and from the university community. In particular, the Geosciences activity provides funding for long-term crosscutting research efforts at national laboratories, which are directly and immediately transferred to the applied programs when needed. The activity also supports the development of research capabilities and communities within both national laboratories and universities that provide manpower for applied programs. The Geosciences activity in BES provides the majority of individual investigator basic research funding for the federal government in areas with the greatest impact on unique DOE missions such as high-resolution Earth imaging and low-temperature, low-pressure geochemical processes in the subsurface.

Scientific Challenges:

Understanding the natural heterogeneity of geochemical and geophysical properties, processes, and rate laws is critical to managing improved production of the Earth's energy resources and safe disposal of energy related wastes. New investigations are needed at the smallest scales studying electronic properties, geochemical reactivity, solute properties, and isotopic distributions in both inorganic and organic systems. Mineral-fluid-microbe systems are also new targets for systematic examination. Understanding pristine natural systems and DOE-specific sites requires improving our capabilities to make and understand high-resolution geochemical and geophysical measurements experimentally and in the field and to model them. Understanding mineral-fluid interactions are key to predicting the fates of contaminants in the environment or predicting nuclear waste-site performance. Improved high-resolution geophysical imaging will underlie new resource recovery, tracking of contaminants, and predicting and tracking repository performance, whether for nuclear or energy-related wastes such as CO_2. Improved imaging and tracking of geochemical processes at the atomic (angstrom) scale using synchrotron x-rays and neutrons is critical for progress in understanding geochemical systems. In addition, new research on high-pressure/high-temperature mineralogical systems will create new opportunities to study and manipulate fundamental mineral and mineral-fluid properties and interactions. Upgrading national laboratory and university investigator experimental, field instrumentation and computational capabilities with new instrumentation and facilities is a continuing challenge. Even with new improved analytical equipment, technical challenges will continue in mastering data-fusion approaches to multiple-technique measurements, such as combined x-ray and neutron analyses or combined seismic-electromagnetic measurements. Computational capabilities driven by the PC-cluster approach with new higher speed chips (3GHz and greater) will enable optimization of clusters for individual molecular dynamics, seismic, electroagnetic, geomechanical, and hydrologic modeling techniques and provide unique support to experimental analysis.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
22,212	20,494	22,345

Performer	Funding Percentage
DOE Laboratories	47 %
Universities	53 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

In the near term, geosciences research continues its basic activity in fundamental rock physics, hydrogeology, analytical geochemistry, and theoretical and experimental geochemistry. It continues national laboratory and university projects focusing on understanding the significance of commonly observed natural nanophases and nanoparticles in shallow earth systems. The activity continues working with various groups on investigating uses of neutrons in Geosciences.

In the mid-term, the activity initiates new research efforts on imaging of earth processes under the Chemical Imaging and Mid-range Instrumentation initiatives, with attention devoted both to improved small-scale imaging (geochemistry focus) using x-ray sources, neutron sources, and scanning microscopy, and large-scale imaging (geophysics focus) of physical properties through understanding intrinsic attenuation within seismic and electromagnetic imaging. New high-pressure/high-temperature research activities begin to investigate how physical and chemical properties in the Earth vary with depth and Earth dynamics. The GSECARS and BESSRC at the Advanced Photon Source (APS) begin their second decade as the premier synchrotron user facilities for the earth sciences community, pioneering approaches that can be exported to other facilities such as the National Synchrotron Light Source II (NSLS II).

In the longer term, Geosciences activities will link analytical capabilities with computational capabilities at the nano-, micro- and macro-scales to provide understanding of geochemical processes occurring at natural time and length scales. Geosciences activities will provide robust understanding of what can be measured remotely at depth by geophysical means, and will increase both the depth of current resolution and the resolution at any depths of interest. Geosciences activities will pioneer the use of neutrons to understand geological processes.

Research Activity: Chemical Energy and Chemical Engineering

Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact(s): Paul H. Maupin (Paul.Maupin@science.doe.gov; 301-903-4355)
Team Leader: John C. Miller
Division Director: Eric A. Rohlfing (Acting)

Portfolio Description:

This activity supports fundamental research in two major research areas: Electrochemistry and Thermophysical Properties. The electrochemistry area addresses the chemical and physical transformations underlying chemical energy storage and conversion and their relationships to limitations in the performance of electrochemical systems. Research activities center on the physics and chemistry of interactions at interfaces between anode, cathode, and electrolytes. The program covers a broad spectrum of fundamental studies of composite electrode structures; failure and degradation of active electrochemical systems; and thin film electrodes, electrolytes, and interfaces to provide fundamental knowledge that will lead to improvements in operating characteristics for electrochemical systems. The program also addresses aspects traditionally of interest to that portion of the chemical engineering community interested in modeling and predicting the thermophysical properties of systems that underpin engineering design activities. This includes studies of thermodynamic behavior, mixing, and physical and chemical rate processes in these systems. Particular attention is given to linked experimental and theoretical aspects of phase equilibria in simple and complex fluids including supercritical phenomena. Also included are fundamental studies of theoretical approaches for understanding thermophysical and thermochemical properties, molecular simulation, and the generation of new equations of states. Emphasis is given to improving and developing the scientific basis for engineering generalizations and their unifying theories.

Unique Aspects:

This activity is the only federal program that supports fundamental electrochemical research as an interdisciplinary program incorporating the disciplines of physics, chemistry, materials science (metallurgy, ceramics, and polymer science), and chemical engineering targeted at understanding the underlying molecular phenomena in electrochemical energy storage and conversion processes and for electrochemical methods useful in analytical chemistry.

Relationship to Other Programs:

Coordination of fundamental and applied research efforts in electrochemistry across the government is accomplished by participation in the Interagency Power Working Group where the program manager is the vice chair of The Chemical Working Group. Within the Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), close coordination with the Battery and Fuel Cell programs in the Office of Transportation Technologies is accomplished through joint program meetings, workshops, and strategy sessions. Coordination in the Chemical Engineering area is primarily with the Chemical Industry Team in the EERE Office of Industrial Technologies through participation in the Chemical Industry Vision 2020 planning activity and the development of joint topics for the Small Business Innovation Research (SBIR) program. A similar relationship with the Fuels program in the Office of Fossil Energy has led to joint SBIR topic development. Additional interaction with the Chemical and Transport Systems Division in the Engineering Directorate at the National Science Foundation is accomplished through direct contact.

Significant Accomplishments:

- Lithium and lithium ion batteries: The most significant accomplishment in electrochemistry research supported by the program was a spin off from early research on the electrochemistry of reactive metals in polar aprotic solvents by the late Charles Tobias of Lawrence Berkeley National Laboratory. It is widely acknowledged that this research (circa 1964) led to the first lithium battery. The same electrolyte solvent systems are still used today in the current generation of rechargeable lithium and lithium ion batteries.
- Replacements for Chlorofluorocarbons (CFCs): Research in thermophysical properties led to the development of an equation of state used in identifying replacements for CFCs that were responsible for destroying the ozone in the stratosphere**.**
- Hydrogen bonding in water: Research in molecular simulation led to clearing up controversial neutron scattering results on the nature of hydrogen bonding in water under supercritical conditions.

- Thin film rechargeable lithium batteries: Research in solid state electrolytes led to a new generation of thin film rechargeable lithium batteries that are about the thickness of saran wrap.
- Room temperature molten salt electrolytes: Research in molten salt electrolytes led to new room temperature systems that are showing promise in reactive metal systems such as sodium and lithium.
- The structural origin of water's anomalous properties: A new formalism for the quantification of structural order in water, based on the introduction of two order parameters has been developed.

Mission Relevance:

Understanding the thermophysical behavior of molecules, mixtures, and solutions under a variety of conditions impacts a large range of energy relevant technologies. In aqueous systems the relevance ranges from steam properties, power production, nuclear reactor technology, geothermal processes, scaling, corrosion, gas hydrates, mineralization, and biochemical processes to industrial processes using aqueous processing. In nonaqueous systems it includes, fuel and chemical processing and manufacturing, natural gas production and use, materials processing and synthesis, and green chemistry. In electrochemistry, understanding what controls electrode and electrolyte performance is key to future improvements in electrochemical components used in nuclear weapons, remote sensing for nonproliferation applications, electronic devices, telecommunications, satellites, solar and wind energy use, electric power production, and electric and hybrid vehicles, as well as advanced electroanalytical chemistry methods.

Scientific Challenges:

As yet, there is not the theory, the computational or experimental ability to understand the role of interfaces in chemical and electrochemical processes. In the electrochemistry area the limited understanding of electrochemistry at the interface of dissimilar solids and phases and at buried interfaces is hindering progress in achieving high power and low cost systems needed in electric and hybrid vehicles, for effective use of wind and solar energy sources, and for distributed power generation by chemical fuel cells. In the chemical engineering area the challenge is a different type of interface, that is, the interface of theoretical and computational methods from the molecular and nanometer scale to the mesoscale where the collective properties of chemical systems impact energy intensive chemical process designs. Efforts to link atomic/molecular properties to colligative properties will continue to be a challenge. In complex liquids the problem is worse. There is not a basic understanding of the liquid state that compares with either the solid or gaseous states.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
11,938	3,731	1,817

Performer	Funding Percentage
DOE Laboratories	49 %
Universities	48 %
Other	3 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

The program provides funding for 40 university grants supporting about 40 students and partially supporting about 45 faculty and senior staff and 7 programs at DOE national laboratories supporting about 15 senior staff and 10 postdoctoral associates. Programs at the national laboratories are multi-investigator efforts on problems that require extensive participation by experienced scientists. These programs usually underscore the user facilities at the laboratories or act as the focal point for specific research efforts vital to the DOE mission. This program supports research of this type at Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory. Many of the research efforts at national laboratories involve interfaces with the university and industrial communities and user facilities.

Projected Evolution: Opportunities deal with the emergence of the ability to control electrode structures on the nanometer scale. Preliminary studies have shown that this has a great impact on the electrochemical efficiency of electrode processes and the rate at which they respond to electrochemical potentials. New funding would capitalize on this new frontier and explore the nature of electrochemical reactions in this new realm. In the thermophysical property focus area, a trend towards greater use of molecular level theory and molecular simulation is increasing the need for increased activities at the interface of computational quantum chemistry and process design in chemical engineering. New funding would address these issues as well and seek to provide a theoretical basis for the incorporation of nanoscale to mesoscale modeling capabilities of importance to the process industries.

Research Activity:	**Structure and Composition of Materials**
Division:	Materials Sciences and Engineering
Primary Contact(s):	Jane G. Zhu (jane.zhu@science.doe.gov; 301-903-3811)
Team Leader:	Helen Kerch (Acting)
Division Director:	Harriet Kung

Portfolio Description:

This activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. Increasingly important are the nanoscale structures and the structure and composition of inhomogeneities including defects, interfaces, surfaces, and precipitates. Advancing the state of the art of electron beam and scanning probe techniques and instrumentation for quantitative microscopy and microanalysis is an essential element in this portfolio.

Unique Aspects:

This activity is driven by the need for quantitative characterization and understanding of materials structure and its evolution over atomic to micron length scales. It is a major source of research in the United States that is focused on structure and defects in atomic configurations over all length scales and dimensionalities, and is the nation's only investment in large-scale, comprehensive microscopy research groups which bring together science-driven investigators whose focus is the development and implementation of a wide variety of electron scattering and scanning probe techniques. Therefore, it supports the facility stewardship role of the Department of Energy (DOE) by enabling full exploitation of the BES three electron microscopy user centers. The portfolio includes characterization and analysis of materials by transmission and scanning transmission electron microscopy, atom-probe field ion microscopy, scanning probe microscopies, spin polarized low energy electron microscopy, electron beam holography and tomography, convergent beam electron diffraction, ultrafast electron diffraction and microscopy, and other state of the art methods. Research results are increasingly coupled with first-principles theory, which offers quantitative insights into the atomic origins of materials properties.

Relationship to Other Programs:

The structure and Composition of Materials program interfaces with other programs in BES, other offices in DOE, and other federal agencies.

BES:
- Coordinated with activities under Mechanical Behavior and Radiation Effects, Physical Behavior, Synthesis and Processing, X-Ray and Neutron Scattering, Condensed Matter Physics, Materials Chemistry and Biomolecular Materials, Catalysis, Electron-beam Microcharacterization Centers, and Nanoscience Centers
- Linked with the Computational Materials Sciences Network

Other offices in DOE:
- Hydrogen Fuel Initiative (HFI)
- Energy Materials Coordinating Committee (EMaCC)

Interagency:
- Interagency Coordination and Communications Group for Metals (NSTC/CT/MatTec)
- Interagency Coordinating Committee on Structural Ceramics (NSTC/CT/MatTec)
- National Nanoscience Initiative (NNI)

Significant Accomplishments:

World class scientific achievements in this program represent the leading U.S. capabilities for structural and compositional characterization at atomic length scale, coupled with advances in detectability limits and precision of quantitative analytical measurement. Accomplishments include:
- The successful correction of electron microscope lens aberrations has doubled resolution in just a few years, allowing for the first time the direct imaging of materials at sub-Angstrom resolution.

- The first spectroscopic imaging of single atoms within a bulk solid using an aberration-corrected scanning transmission electron microscope. The ability to collect electron energy loss spectra from an individual atom allows not only elemental identification, but also the determination of chemical valence and its bonding configuration or local electronic structure through analysis of the fine structure of the spectroscopic absorption edge.
- Combined scanning probes, electron microscopy, and theoretical calculations to reveal an unexpected behavior: ferroelectric ordering in a non ferroelectric compound ($SrTiO_3$) induced by a grain boundary.
- Invented new local probes: scanning impedance microscopy and nanoimpedance spectroscopy.
- Developed advanced computer processing methods for a through-focus series of electron microscope images to achieve an "information limit" that exceeds the resolution of the best-ever single optimal image. This method enabled the first imaging of the light non-metallic elements-carbon, nitrogen, and oxygen.
- Developed a new interferometric electron beam technique to measure atomic displacements in crystals with unprecedented picometer accuracy.
- Developed and demonstrated new quantitative methods to image and measure the distribution of valence electrons in solids, which have made significant contributions to the understanding of electronic transport in high temperature superconductors.
- Conceived and constructed the first three-dimensional, energy compensated, position sensitive atom microprobe that permits compositional imaging and depth analysis with atomic resolution.
- Refined Atomic Location by Channeling Enhanced Microanalysis in an electron microscope to precisely define locations of various atomic elements and reveal an unprecedented level of information in a variety of technologically important alloys.
- Pioneered the application of electron beam holography to image and measure the grain-boundary potentials in vital ceramics such as superconductors, ferroelectrics, and dielectrics by exploiting the sensitivity of highly coherent electron waves to local electric fields.
- Developed the highest spatial resolution and lowest elemental detectability limit in-situ electron energy loss spectroscopy.
- Developed a new electron microscopy technique known as "fluctuation microscopy" that shows atomic arrangements in amorphous and glassy materials better than any alternative method.
- Incorporated a controlled nanoindentation apparatus within a transmission electron microscope for the first time, permitting the simultaneous atomic-scale observation and mechanical testing of nanoscale sample regions.
- Developed the "Embedded Atom Method" that revolutionized the field of computational materials science by permitting large-scale simulations of atomic structure and evolution. It is currently being used by more than 100 groups worldwide and has resulted in over 1100 published works with over 2700 citations to the original work.

Mission Relevance:

The fundamental properties of materials used in all areas of energy technology depend upon their structure and composition. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon these characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g., dislocations, grain boundaries, interfaces, magnetic domain walls, and precipitates) determine and control critical behaviors such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, superconducting parameters, magnetic behavior, and corrosion susceptibility. Quantitative analysis of nanoscale structures is crucial to the progress of nanoscale science–a major thrust in BES. The program is also relevant to the DOE HFI through the structural determination of nanostructured materials for hydrogen storage and solar hydrogen generation.

Scientific Challenges:

Major scientific challenges in the Structure and Composition of Materials program are: quantitative analysis of nanoscaled structures in nanomaterials, including the atomic, electronic, and magnetic structures; understanding nanoscale interactions and phenomena; understanding correlation between electrons and spins at nanoscale; determination of interface structures between dissimilar materials; understanding the role played by the interface structure in the evolution of microstructures; determination of local inhomogeneity and structure disorder; understanding the link between interface/surface/defect structures and materials properties; understanding of the structure and dynamics of amorphous materials, especially the short- and long-range order effects; development of ultrafast electron microscopy with high resolution both spatially and temporally to study the atomic level mechanisms during structural transformations; developing the ability to measure the distribution of valence electrons with sufficient accuracy; and the application of first principles theory to understand and predict the structures of real materials. To address these challenges, new state-of-the-art experimental and theoretical techniques will need to be developed. It is our long term goal to invent multiscale characterizations tools and be able to link structural evolution, dynamics, and electronic behavior with first principles understanding of structure.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
24,907	16,943	22,245

Performer	Funding Percentage
DOE Laboratories	77%
Universities	23%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

In the near term, program evolution builds upon recent accomplishments that span a wide range of areas including advances in microcharacterization science, the characterization of nanostructured materials, and detailed models of magnetic and structural phenomena. Electron scattering and scanning probe approaches supported by this program have higher spatial resolution than most other materials characterization techniques and are thus unique in their ability to characterize discrete nanoscale and nanostructured regions within the interiors of samples. Characterization of semiconducting, superconducting, magnetic, and ferroelectric materials benefits greatly from these abilities and from other research supported in this program. Concurrently, new frontiers in characterizing and understanding the microstructure and microchemistry of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron microscopy techniques will be continued, which will be partnered with the three electron-beam microcharacterization centers that were built up in this program and are now in the Electron Beam Microcharacterization activity. The enormous improvement in sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of atomic-scale tomography, single-atom spectroscopic detection and identification, and increased experiment volumes within the microscope and consequently greater in-situ analysis capabilities (under perturbing parameters such as temperature, irradiation, stress, magnetic field, and chemical environment).

New methods and approaches addressing the scientific challenges will lead to the development of unique new analysis tools and breakthroughs in materials. The combined new experimental and theoretical capabilities will enable the fundamental understanding of atomic origins of materials properties. Significant advances will be made in the detailed understanding of the mechanisms by which grain boundaries, interfaces and defects in metals, ceramics, semiconductors, and polymers influence the properties and behavior of these materials. Implementing nanostructural control over these mechanisms will revolutionize the fundamental principles of materials design.

Research Activity: Mechanical Behavior and Radiation Effects

Division: Materials Sciences and Engineering
Primary Contact(s): Yok Chen (yok.chen@science.doe.gov; 301-903-4174)
Team Leader: Helen Kerch (Acting)
Division Director: Harriet Kung

Portfolio Description:

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials with an emphasis on the relationships between mechanical behavior and radiation effects and defects in the material. This research builds on atomic level understanding of the relationship between mechanical behavior and defects in order to develop predictive models of materials behavior for the design of materials having superior mechanical behavior such as at very high temperatures. The mechanical behavior of materials under repeated or cyclic stress, high rates of stress application, and over a range of temperatures and stress conditions are relevant to present and projected energy conversion systems. The focus on radiation effects is to achieve atomic level understanding of radiation damage mechanisms and subsequent materials property changes to design radiation-tolerant materials for advanced energy systems. Important radiation induced materials property changes include embrittlement, stress-corrosion cracking, amorphization (transition from a crystalline to a non-crystalline phase), and ion irradiation-induced surface modification.

Unique Aspects:

The ability from a fundamental basis to predict materials performance and reliability and to address service life extension issues is important to the Department of Energy (DOE) missions in fossil energy, fusion energy, nuclear energy, energy efficiency, radioactive waste storage, environmental management, and defense programs. Among the key materials performance issues for these technologies are load-bearing capability, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility and deformability, and radiation tolerance. This activity represents a major fraction of federally supported basic research in mechanical behavior and is the sole source of basic research in radiation damage. In the science of mechanical behavior, cutting-edge experimental and computational tools are bringing about a renaissance, such that researchers are now beginning to develop unified, first-principles models of deformation, fracture, and damage. The compelling need for understanding deformation mechanisms is related to the fact that virtually all structural metals used in energy systems are fabricated to desired forms and shapes by deformation processes. The compelling need in radiation effects - for valid predictive models to forecast the long-term degradation of reactor components and radioactive waste hosts - is expected to become increasingly critical over the next decade. Radiation tolerance of structural metals and insulating ceramics is also a matter of great concern for fusion energy systems.

Relationship to Other Programs:

This activity interacts closely with the DOE programs in fossil energy, fusion energy, nuclear energy, energy efficiency, radioactive waste storage, environmental management, and defense programs especially in the areas of materials performance and reliability. Through its focus on atomic level understanding of defect-property relationships it is complementary to the emphasis on behavior of complex materials in the Physical Behavior of Materials activity and Structure and Composition of Materials research whose focus is on the relationship of structure to physical properties. Similarly, the radiation effects element's activity on radiation-tolerant materials complements Heavy Element Chemistry research whose focus is on actinide and heavy element chemistry. Principal investigators use BES national user facilities for x-ray and neutron scattering and collaborate with the X-ray and Neutron Scattering activities. They also use the BES Electron Beam Microcharacterization Centers and the Nanoscale Science Research Centers.

Significant Accomplishments:

Atomic Scale Revelations of Brittle Fracture. A molecular dynamics study has revealed for the first time how fracture processes at the atomic scale affect bulk behavior, such as dynamic fracture toughness and crack propagation rate. Using an interatomic potential derived from the modified embedded atom method, atomistic calculations showed that at low crack propagation rates, silicon fractures via perfect cleavage on atomic planes, but at higher crack propagation rates, atomic lattice defects, uneven crack surfaces, and phonon vibrations are produced leading to an increase in the energy consumed during fracture. This increased energy consumption reduces the energy that would otherwise be available to drive cracks to even higher propagation rates and limits the maximum crack propagation rate to significantly less than the theoretical maximum crack propagation rate. The results demonstrate that molecular dynamics can be used to accurately reproduce bulk experimental results, while simultaneously capturing the atomic level details of the fracture process. The added significance of this method is that it can be easily extended to other materials and incorporated into models of large dynamic systems.

Silicon Carbide: Going Where Silicon-based Technology Cannot Go. Major breakthroughs in understanding atomic defects and nanostructures in silicon carbide enable this semiconductor material to be used in a new generation of devices for severe environments where silicon-based devices cannot operate. This new understanding can be used to overcome materials degradation problems that hinder advanced device development. Atomistic computational methods have determined critical defect formation and diffusion properties and accurately predicted evolution of nanostructures, phase transformations, and changes in volume and mechanical properties. The excellent agreement between computational predictions and experimental measurements provides the scientific confidence to use the computational methods to predict properties and behavior under extreme conditions that cannot be tested in the laboratory. It allows the use of defect engineering to minimize degradation, enhance materials reliability, and design materials that allow the remarkable physical properties and biocompatibility of silicon carbide to be fully used for energy-saving devices, advanced optoelectronics, improved sensors, medical devices, advanced-energy components, and chemically-challenging environments.

Mechanical Properties Affected by Magnetic Interaction - A New Fundamental Principle. Quantum effects involving magnetic interaction have been discovered to be responsible for unexpected solid solution hardening/softening in intermetallic alloys, thus resulting in their superior mechanical properties. This new phenomenon was discovered by careful coordination between theory and experiments: first-principle quantum-mechanical calculations coupled with polarized neutron diffraction and electron energy-loss spectroscopy (EELS). Experimental studies have revealed unusual interatomic spacing and resultant solid solution softening in nickel-aluminum alloys induced by iron, manganese and chromium solute atoms, which cannot be explained by current hardening theories. Quantum mechanical calculations revealed the development of a large electron-spin polarization when these solute atoms substitute for aluminum in nickel-aluminum alloys. The spin polarization results in a large magnetic moment that dilates the lattice parameter and strongly affects mechanical properties of nickel-aluminum alloys. The calculated values are unambiguously supported by EELS and polarized neutron diffraction. These studies have led to the discovery of a new concept in the design of strong and tough intermetallic and metallic alloys for advanced heat engines and energy conversion systems. This new principle is expected to appear in textbooks illustrating cross-fertilization between two disciplines which have had no connection.

Mission Relevance:

The scientific results of this activity contribute to the DOE mission in the areas of fossil energy, fusion energy, nuclear energy, transportation systems, industrial technologies, defense programs, radioactive waste storage, energy efficiency, and environmental management. In an age when economics require life extension of materials, and environmental and safety concerns demand reliability, the ability to predict performance from a fundamental basis is a priority. Furthermore, high energy-conversion efficiency requires materials that maintain their structural integrity at high operating temperatures. It is also necessary to understand the deformation behavior of structural metals so as to fabricate them to desired forms and shapes. This activity seeks to understand the mechanical behavior of materials. It also relates to nuclear technologies including fusion, radioactive waste storage, and extending the reliability and safe lifetime of nuclear facilities. For example, a recent study to understand environmental cracking of metallic alloys on the atomic scale has strong implications in pressurized water reactors.

Scientific Challenges:

Amorphization of materials occurs at the atomic scale when oxides are irradiated with neutrons or positive ions, adversely affecting its physical and chemical properties. By understanding the mechanism and the parameters contributing to radiation tolerance, it will be possible to predict or engineer materials that are less susceptible to amorphization by radiation damage. Dislocation theory for deformation and fracture is typically valid for length scales less than 0.1 micron. Continuum elasticity and constitutive equations derived from it are typically limited to macroscopic length scales greater than 10 microns. These models do not converge in the interval often referred to as “mesoscale” between these limits. It is often possible, however, to control or "tune" microstructural features in this mesoscale regime by suitable adjustment of synthesis and processing parameters. Thus a unified model is sought that will quantitatively describe mechanical behavior (including strength, deformation parameters, and fracture toughness) over all length scales. Such a model could be used to design microstructures as well as synthesis and processing parameters leading to optimized materials properties and behavior. Many metals and metallic alloys, including common steels, undergo a profound ductile-to-brittle transition over a small temperature interval, without detectable structural or chemical change. The understanding of the origins of this transition remains elusive and represents an on-going challenge. Investigating and understanding nanoscale materials, their response to mechanical stress and radiation damage, will reveal previously inaccessible realms of materials behavior as well as paving the way to novel applications.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
14,008	13,037	18,195

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

Research opportunities that can be realized by the application of mechanics fundamentals to the general area of self-assembly, directed self-assembly, and fluidics will constitute an increasingly significant part of the technology that mass-produces devices that harvest energy, sense trace amounts of matter, and manipulate information. Mechanics plays a fundamental role in understanding functions in biological, bio-inspired, and bio-hybrid material systems at all length scales. Biology and biological techniques are just beginning to be used to develop new materials and devices that will have broad impacts on engineering. An understand is needed of how the hierarchical nano- and micro-structure of biological of soft materials controls the deformation and fracturing modes and behaviors of the biological systems. This understanding needs to be imported to the behavior of hard alloys and ceramics that are used in the hostile environment of energy systems. With the emerging importance of nanoscale structures with high surface-to-volume ratios, many of the old unresolved topics, such as fragmentation and shear instabilities, need to be revisited from a multi-disciplinary perspective, taking advantage of more powerful parallel computational platforms and new experimental tools.

The accessibility of national user facilities for neutrons and photons enables a new dimension for the studies of mechanical behavior of materials. The advantages of using neutrons and photons, as compared to the more traditional electron scattering techniques, such as in transmission electron microscopy, are several including in-situ and non-destructive experiments on bulk samples, time-resolved studies, and three dimensional profiles.

Unified models will be developed covering all length scales that will provide significant insights into deformation and fracture. Concurrent advances in microstructural characterization will be exploited to understand the ductile-to-brittle transition and permit this understanding to be exploited for the design of embrittlement-resistant materials. The origins of radiation tolerance will continue to be pursued including exploitation of parameters, which feed into the phenomena of radiation tolerance, such as structure, stoichiometry, and ionic (or atomic) size. Mesoscale and nanoscale modeling efforts will be extended to include nanostructured materials.

With high-end computational capability now a reality, computational materials science will play a pre-eminent role in predicting radiation-damage evolution in materials. Specific research for materials relevant to future fusion and Generation-IV fission reactors will examine methods to examine structural materials performance issues. The need to predict material behavior under exposure conditions (irradiation, temperature, and mechanical loading) that represent a significant extrapolation beyond our existing knowledge base will also be addressed.

Research Activity: Physical Behavior of Materials
Division: Materials Sciences and Engineering
Primary Contact: Refik Kortan (Refik.Kortan@science.doe.gov; 301-903-3427)
Team Leader: Helen Kerch (Acting)
Division Director: Harriet Kung

Portfolio Description:
This activity is a fundamental research program focusing on the functional properties of materials. The major emphasis is on the behavior of complex materials in response to external stimuli often encountered in energy-intensive applications. This basic research program focuses on physical responses (such as optical, electronic, or magnetic changes) to temperature, electro-magnetic fields, chemical environments, and the proximity effects of surfaces and interfaces with an emphasis on the relationships between physical behavior and the microstructure and defects in the material. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the semiconducting, superconducting and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures in energy conversion processes; and diffusion and transport phenomena in ceramic electrolytes for improved performance in batteries and fuel cells. Basic research is also supported to develop new instrumentation, including in-situ experimental tools, to probe the physical behavior in real environments encountered in energy applications.

Unique Aspects:
Research in this activity provides the primary support of the fundamental understanding and identification of detailed mechanisms responsible for the physical behavior of materials, and the incorporation of this knowledge into reliable detailed predictive models. The understanding that has resulted from such modeling work has already led to the design of unique new classes of materials including compound semiconductors, tough structural ceramics, ferroelectrics, and magnetocaloric materials. Some specific examples include: new levels of magnetic properties from nanoscale clusters, compound semiconductors that can remove excess CO_2 from the atmosphere, highly desirable phases of ferroelectric materials that can be formed through novel processing techniques, and a breakthrough in understanding of the chemistry of friction enabling the tuning of lubrication layers.

Relationship to Other Programs:
BES:

- Closely linked with activities under Engineering Physics, Structure and Composition, Mechanical Behavior and Radiation Effects, Synthesis and Processing Sciences, X-ray and Neutron Scattering, and Condensed Matter Physics
- Linked with Center of Excellence for Synthesis and Processing of Advanced Materials
- Linked with Computational Materials Sciences Network

Other Parts of DOE:

- Solid State Lighting/Building Technologies Program, Office of Energy Efficiency and Renewable Energy
- Nuclear Energy Research Initiative
- Energy Materials Coordinating Committee
- Hydrogen Coordinating Committee

Interagency:

- Interagency Coordination Group on Metals (NSTC/CT/MatTec)
- Interagency Coordination Group on Structural Ceramics (NSTC/CT/MatTec)
- Interagency Coordination Group on Nondestructive Evaluation (NSTC/CT/MatTec)
- Interagency Working Group on Nanotechnology (NSTC/CT/MatTec)
- OSTP Interagency Coordination Group on Hydrogen

Significant Accomplishments:

This activity has had broad and significant impact in many classes of materials and phenomena. In magnetic materials, continuous fundamental studies of bulk alloys and nanoclusters have led to the following breakthroughs:

- Discovery of the extraordinary giant magnetocaloric phenomena, which has led to the demonstration of high-efficiency refrigeration that does not require the use of any refrigerant. This technology completely eliminates ozone depleting chemicals (e.g., Freon) used by conventional refrigeration and has the potential to develop into a global market.
- Development of ferromagnetic bulk metallic glasses with dramatic reductions in hysteretic energy loss, which has the potential of leading to $30 billion dollars per year in savings in improved energy efficient motors and transformers.
- The prediction and validation of extremely large magnetic moments in nanoclusters, which has the potential of leading to higher density nanomagnetic storage devices.

In semiconductors, major research accomplishments in silicon-based and other compound semiconductors are:

- Developed a biocompatible semiconductor laser for the rapid detection and analysis of chemical agents, such as anthrax spores. The device was based on recent advances in the surface chemistry of semiconductors and the concept of quantum squeezing of light emitted through a spore flowing at high speed in the laser's microcavity. This field-deployable biolaser should be able to identify different types of spores (e.g., anthrax) within a large population of harmless spores rapidly and effectively.
- Through research in wide band-gap semiconductors achieved a succession of world records for energy conversion efficiency in solar photovoltaics and been recognized by the 2001 John Bardeen Award from the American Physical Society.
- Developed a new dielectric technology for capacitors, based on high dielectric constant ceramic perovskites oxides. The new technology overcomes the conventional silicon dioxides thickness limitation of two to three nanometers (three to five atomic layers), and thus offers promise of further extending Moore's Law which predicts the doubling of the performance/cost ratio for silicon-based devices every eighteen months. This breakthrough promises smaller, faster field effect transistors leading to faster and more versatile computers.
- Achieved a tenfold increase in the electrical conductivity of the semiconductor gallium arsenide which is now attracting market interest for application in electronic devices, diode lasers, reading compact discs, and ultra-high speed transistors.
- Achieved a new milestone towards light-emitting silicon through the identification of oxygen atoms as the mediator of silicon energy states. The result suggests possible ways to enhance light emitting efficiency of silicon, and hence easier and cheaper ways to integrate optoelectronic components with silicon-based technology.

Other major accomplishments supported by this activity are:

- A "direct" visualization of the three-dimensional rearrangements of atoms in a crystal lattice triggered by a magnetic field was realized by an *in-situ* x-ray diffraction technique. The observation sheds light on the mechanism governing the magnetocaloric effect and paves the way to designing advanced materials for improved environmentally-friendly cooling technologies.
- Two-dimensional (2D) photonic band gap crystals in the visible wavelength have been fabricated based on the self-assembled periodic arrays of aligned carbon nanotubes. These aligned periodic carbon nanotubes are unique as they exhibit a "tunable" photonic bandgap not previously observed in the visible region and demonstrate the feasibility of fabricating large areas of 2D photonic crystals without sophisticated electron lithography procedures. These photonic crystals may find wide applications in optical signal processing and switching.
- A synergistic approach of combined photoelectron spectroscopy and quantum chemical calculations has provided crucial insights on the origin of the loss of nobility and the catalytic properties of nanoscale gold particles.
- An innovative visualization tool has provided new insights in the corrosion behavior of aluminum and its alloys. The results show that the "noise" from electrical signals is dominated by the pit growth processes as opposed to the initiation and re-passivation of protective oxides speculated previously and observed in stainless steels.
- Strong coupling and giant magnetic moments were predicted in manganese atom clusters in the presence of nitrogen. The predictions are consistent with recent experimental results and the finding will aid the design of new magnetic materials and novel spintronic devices.
- Novel zinc oxide nanostructures, including hierarchical structures with different symmetries, nanobridges, and nanowalls have been synthesized by an innovative vapor transport and condensation technique. The results

demonstrate the feasibility of joining two different nano-components into a hierarchical structure. The nano-composites exhibited superior electrical and thermal conductivities.

- Russian doll models for the stabilization of silicon cage structures found that unfavorable energetics in the stretching of silicon to silicon bonds were responsible for previous failed attempts to synthesize the 60-atom silicon structure.
- A new epitaxial liquid-assisted growth method, which involves a fluoride compound in precursor films, has been developed to grow thick films of superconducting YBCO. The study yielded an understanding of the complex and unconventional growth process, which involves reactions of precursor films to form the desired compounds in several sequential steps. The understanding can be extended to other technologically important oxides that are of critical importance in solid-state electronic devices.
- Nanocrystals of semiconductor cadmium selenide were demonstrated to successfully remove excess carbon dioxide from the atmosphere. The technology could potentially convert unwanted carbon dioxide into useful organic molecules with major environmental benefits.
- Experimental studies of interfacial forces have resulted in an atomic understanding of interfacial adhesion and the ability to tune frictional forces at the atomic level. The development of instrumentation that enabled this work was recognized by an R&D 100 award.
- Pioneering work in rare earth alloys, recognized by another R&D 100 Award, has led to high performance phosphors that are now marketed in television tubes, and cheaper and more powerful permanent magnets, including the development of a new market and the spawning of a private sector company that markets it.
- A new wetting model was constructed and validated by recent AFM observations of the interfacial structures between molten metals and ceramic surfaces. The model takes into account diffusion of the solid substrate under the molten metal and successfully explains why the contact angle differs for droplets that are growing versus those that are evaporating. Understanding the behavior at these metal-ceramic interfaces is critical to improving various industrial processes including soldering, brazing, coating, and composite processing.
- An innovative approach enabled the first direct observation on how water behaves near a hydrophobic surface. Measurements made by the surface force apparatus revealed the thrashing and rippling behavior of water near hydrophobic surfaces. These insights open doors to understanding a wide range of biological dynamic processes from protein folding and enzyme reactivity.
- A new study confirms the theoretical analysis that molecules of hydrogen, oxygen, and even water can travel across conducting membranes in opposite directions from what would normally be expected from chemical potential gradients. The new analysis shows that the behavior is a result of the simultaneous, coupled transport of multiple conducting species. The understanding of membrane transport is important in the development of advanced materials for energy storage such as fuel cells.

Mission Relevance:

Research underpins the DOE missions by developing the basic science necessary for improving the reliability of materials in chemical, electrical, and electrochemical applications and for improving the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, and hostile chemical conditions), understanding how their behavior is linked to their surroundings and treatment history is critical. Research in mission-relevant topics in this activity include corrosion, which annually consumes 4.2 percent of the Gross National Product; photovoltaics; fast-ion conducting electrolytes for batteries and fuel cells; novel magnetic materials for low magnetic loss and high-density storage; and magnetocaloric materials for high-efficiency refrigeration. The photovoltaic research supported is complementary to Experimental and Theoretical Condensed Matter Physics, whose emphasis is on the electronic structure of solar conversion processes and systems. Significant interactions and collaborations exist between this activity and Materials Chemistry and Biomolecular Materials program in surface chemistry and electrochemistry as related to oxidation and corrosion research.

Scientific Challenges:

The challenge in this area is to develop the scientific understanding of the mechanisms that control the behavior of materials and to use that understanding to design new materials with desired behaviors. The program encompasses efforts aimed at understanding the behavior of organic and inorganic electronic materials, magnetism and advanced magnetic materials, manipulation of light/photonic lattices, corrosion/electrochemical reactions, and high-temperature materials behavior through intimately connected experimental, theory, and modeling efforts leading to a-priori design of new materials.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
25,551	24,677	29,756

Performer	Funding Percentage
DOE Laboratories	77%
Universities	23%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

In the near term, four central topics define the current program: electronic and magnetic behavior of materials; corrosion and electrochemistry science; nano-scale phenomena; and multiscale modeling of materials behaviors. Major efforts in these areas will continue. Increased investment in organic electronic materials will be considered. In addition, focus in theory and modeling at universities and national laboratories, taking advantage of the vast advances in computing speed and power, will be emphasized.

In the mid- to long-term, in order to understand the macroscopic behavior of materials it is important to understand the relationship between the material's structure and its response to external stimuli. One needs to first study the structure over all length scales, with emphasis at the atomic level, and to understand the response of the nanometer and larger features of the material to those external stimuli. Studies of the physical response of a single nanometer-scale feature needs to be related to the macroscopic behavior of the material. This can often be done with modeling but further advances are necessary to fully couple the length scales from atomic to macroscopic. Currently, atomistic simulation methods can be used to study systems containing hundreds of thousands of atoms, but these systems are still orders of magnitude too small to describe macroscopic behavior. Continuum methods, typically using finite element methods, fail to adequately describe many important properties because they use phenomenology that has little connection to the real processes that govern physical interactions. Modeling at an intermediate length scale, the mesoscale, where many defects can be included and from which predictive models at the continuum scale can be developed is required for advances in materials science. At this intermediate length-scale it is necessary to model the collective phenomena that include well over a billions atoms. Developing and applying novel techniques to these problems will be emphasized in coordination with the investment in theory and modeling. In addition, tremendous advances in organic-based electronic materials applications have been reported recently. This program seeks to foster theory, modeling and simulation activities that address the following key topics in organic electronic materials: charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics.

Finally, in order to understand the complex phenomena that are linked to both a material and its local environment, a long-term investment is needed. During this funding period, we anticipate supporting programs that apply advances in both experimental techniques and computational methodologies to understand the macroscopic behavior of materials by studying materials at all length scales and multiple time scales. In particular, bridging models covering the mesoscale (covering phenomena in the range of 0.1 to 10 microns) will be developed. This is vital to linking disparate length scales and creating a scientifically rigorous understanding of materials performance and behavior. It is also vital to link the time scales that correspond to fast reactions and relaxation processes in materials.

Research Activity: Synthesis and Processing Science

Division: Materials Sciences and Engineering
Primary Contact(s): Timothy Fitzsimmons (Tim.Fitzsimmons@science.doe.gov; 301-903-9830)
Team Leader: Helen Kerch (Acting)
Division Director: Harriet Kung

Portfolio Description:

This activity supports basic research in synthesis and processing science for innovative synthesis of new materials with desired structure, properties or behavior; to understand the physical phenomena which underpin materials synthesis such as diffusion, nucleation and phase transitions; and to develop in situ monitoring and diagnostic capabilities. Examples of activities in synthesis and processing include: (1) the physics of growth of complex thin films and nanoscale objects with an emphasis on atomic layer-by-layer control; (2) preparation techniques for novel single crystal and bulk materials having novel nanoscale attributes; (3) understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and (4) low energy processing techniques for large scale nanostructured materials. This activity includes the operation of the Materials Preparation Center at the Ames Laboratory, which develops innovative and superior processes for materials preparation and provides small quantities of research grade, controlled purity materials and crystals that are otherwise not available to academic, governmental, and industrial research communities for research purposes.

Unique Aspects:

- The Materials Preparation Center (MPC) at the Ames Laboratory is operated for the purposes of understanding and further developing innovative and superior processes and for providing small quantities of unique, research-grade materials that are not otherwise available to academic, governmental, and industrial research communities.
- World-leading thin-film growth capabilities reliant on in situ diagnostics have been developed for the synthesis of thin-films.
- Bulk phase transitions and transformations underlying the advancement of materials process science are studied using highest purity materials, in situ characterization techniques, and simulations.

Relationship to Other Programs:

This program is intimately related to the other research activities in the BES Materials Sciences and Engineering Division as the synthesis and processing of materials is a critically important area of materials research and development. The MPC specializes in the preparation, purification, and fabrication of high-purity rare earth metals, refractory metals, alkaline earth metals, alloys in single crystal and polycrystalline form, metal powders, and metallic and ceramic coatings. The MPC has responded to over 3800 requests for specialty materials preparation and characterization services to academic, government, and industrial research laboratories since its establishment in 1981. The facilities and capabilities of the MPC are also made available to further understanding of process science on the basis of user proposals.

Additional linkages include:
Department of Energy (DOE)

- Office of Energy Efficiency and Renewable Energy (EERE)/Building Technologies/Solid State Lighting/Joint Contractor's Meeting/ February 1-3, 2006
- EERE/Transportation Technologies/Hydrogen Contractor's Meeting, May, 2006
- Energy Materials Coordinating Committee (EMaCC)

Interagency

- Interagency Working Group on Hydrogen
- Interagency Working Group on Manufacturing
- DOE lead on Nanomanufacturing
- MatTec Communications Group for Metals
- MatTec Communications Group for Structural Ceramics
- National Nanotechnology Initiative (NNI)

Significant Accomplishments:

This program has changed the way people understand and think about the preparation of materials. Experimental, theoretical, and computational tools are developed and applied to advance the scientific understanding of complicated thermodynamic and kinetic phenomena underlying processes ranging from self-assembly to far-from-equilibrium reactions that take place in welding. In the epitaxial growth area, a new technique has been developed to deposit ultrathin metallic layers on oxide, which will help next-generation computers boot up instantly by making entire memories immediately available for use. The thin metal layer achieves epitaxial crystallinity after the deposition of only a few atomic layers. This process should be applicable to a wide range of metals on metal oxides. Significant progress has been made in the growth of single crystalline thin films of ferroelectric and ferromagnetic oxides using the molecular-beam epitaxy technique. New candidate ferromagnetic semiconductors have recently been grown by doping transition-metal oxides with magnetic impurities, which are nontraditional but strongly magnetic and thermally robust diluted magnetic semiconductors. Recent breakthroughs in the synthesis of complex oxides have brought the field to an entirely new level, at which complex artificial oxide structures can be realized with an atomic-level precision comparable to that well known for semiconductor heterostructures. Not only can the necessary high-quality ferroelectric films be now grown, but ferroelectrics can be combined with other functional oxides, such as high-temperature superconductors and magnetic oxides, to create multifunctional materials and devices. The shrinking of the relevant lengths to the nanoscale produces new physical phenomena.

New techniques, developed to measure local electromagnetic properties, now permit a fundamental understanding of the mechanism by which solid-solid interfaces and crystalline defects control the behavior of nanostructured as well as macroscopic materials. For the first-time, suppression in dielectric-constant has been observed directly at grain boundaries, contradicting traditional assumptions generally made about grain-boundary behavior, using scanning impedance microscopy and nano-impedance spectroscopy. In the welding area, a coupled thermodynamic and kinetic model was developed to describe stability of the principal phases in stainless steels. This knowledge has led to the modification of the standard diagram used to choose welding electrode compositions for stainless steels. Additional modeling efforts using massively parallel computers have permitted the linkage of macro- and microscopic scale phenomena during the melting and solidification of a weld. This permits simulation and visualization of weld microstructure as a function of processing conditions, e.g., during the melting, addition of new compounds, and resolidification that occurs during welding. Experimentally, tracking of real-time phase transformations that occur during weld solidification was made possible using synchrotron radiation and provided invaluable data to support scientific modeling and simulation leading to better electrode design. Recognitions include the recipients of the Spararagen Award and the Warren F. Savage Award from the American Welding Society.

Other achievements include:

- Investigations of self-assembled heteroepitaxial semiconductor quantum dots using real-time stress sensing and light scattering showed how elastic repulsion determines evolution of dot arrays. Repulsion promotes spatial ordering, accelerates ripening kinetics, and enhances quantum dot phase transition.
- In the self-assembly area, developing scientific understanding of surfactant interactions with ceramic compounds and other materials, including biological tissues, has permitted the growth of ordered porous ceramic structures with hierarchical architecture spanning from the nano- to the macro-scale.
- A rapid, efficient self-assembly process for making nanophase composites that mimic the complex construction of seashells was developed resulting in a strong and tough (crack resistant on impact loading) material.
- Ceramic substrates were synthesized with tailored and regularly ordered nanoscale pores of controlled shapes and sizes. These substrates were found to remove deadly heavy metals such as mercury, lead, and silver from contaminated water.
- A breakthrough in the fundamental understanding of the processing of ceramic aerogels led to a new, non-toxic, low temperature, and low-pressure process to produce films in an environmentally benign manner. This discovery overcame the sixty-year barrier to the large-scale commercial use of these films, won the prestigious Iler Award of the American Chemical Society and was cited as an important discovery by the Wall Street Journal.
- The Materials Preparation Center has completed over 3800 requests for specialized materials preparation and characterization services since its establishment. In addition to the previously mentioned accomplishments, MPC has enabled the technologies of (1) lead free solder, (2) magnetocaloric gadolinium-silicon-germanium alloys, (3) recyclable lightweight automotive composite materials, and (4) Terfenol-D, a mangetostrictive alloy

containing terbium, dysprosium, and iron that was developed at the cCenter and led to the spin-off of a new private sector company which markets this material.

- Quasicrystal coatings produced by plasma-arc spray that have superior wear resistance and thermal insulation behavior coupled with reduced surface friction for potential thermal barrier wear resistant coating applications in aircraft-engine components.
- A uniform three-dimensional coating process known as "Plasma Ion Immersion Processing" was improved so as to fabricate hard coatings, such as diamond-like carbon, that exhibit low sliding friction and superior wear resistance. This process is cost-effective and achieves a high rate of implantation over a very large surface area with uniform thickness and coating quality over complex three-dimensional geometries.
- A nanophase molecular template method was developed to synthesize films that exploit the dielectric properties of air to achieve ultra-low dielectric constants for the next generation of microelectronic devices and computers.
- A unified, fundamental understanding of the multifaceted behavior of H in Mg-doped, p-type GaN was developed that, in several respects, goes beyond what has previously been achieved for H in compound semiconductors. These studies represent a new level of quantitative understanding of hydrogen behavior within compound semiconductors.
- Investigation of the dynamics of self-assembled supramolecular organic oligomers, polymers, and metal chelate systems has revealed methods to control both intra- and intermolecular interactions leading to systems with tunable optical properties.

Mission Relevance:

This research supports DOE overarching goals for improved energy efficiency, protection of the environment, and the advancement of scientific knowledge. Specific relevant applications include discovery of new materials for efficient energy production and use; hard and wear resistant surfaces to reduce friction and wear; high-rate, superplastic forming of light-weight, metallic alloys for fuel efficient vehicles and other structures needed in land and air transportation applications; high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools, bearings, engines, and turbines (to enable fuel efficiency and low-pollutant emissions); ordered intermetallic alloys for harsh applications (requiring heat, load, wear, and corrosion resistance), including engines and turbines (also to enable fuel efficiency and low pollutant emissions); response of magnetic materials to applied static and cyclical stress; plasma, laser, and charged particle beam surface modification to increase corrosion and wear resistance; and welding and joining, including dissimilar and non-metallic materials.

Scientific Challenges:

Understanding the physics and chemistry of the synthesis and processing, as well as the thermodynamics and kinetics of reaction, of nanoscale materials and structures and the elements of the processing environment are critical to the preparation of larger components. There are significant experimental, theoretical, and computational challenges in understanding what is occurring so that the benefits of nanoscale phenomena can be realized in larger scale components. Major scientific challenges also remain in the fabrication and the fundamental understanding in the non-trivial assemblies of inorganic, organic, composite, and biomimetic materials. There is a need for creative and innovative methods to investigate complex systems, such as composite materials with multifunctionality.

Future efforts are required to synthesize new materials for the advancement of science and technologies, to gain the fundamental understandings for better control of materials manipulation and properties, and to solve materials problems, such as adhesion and stability under thermal and environmental stress. Although there is steady progress in the synthesis and processing of materials, there still exists a serious deficit in the ability to produce (new) materials with desired properties and microstructures by rational design and synthesis. Experimental methods and theoretical models need to be developed to achieve mesoscopic structures via various methods, such as self-organized and directed growth. Scientific challenges also lie in new composite materials with various matrices, and in ecologically-benign materials.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
15,149	17,083	21,022

Performer	Funding Percentage
DOE Laboratories	60%
Universities	40%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

- Increased emphasis on understanding the opportunities and challenges presented by nanoscale materials and by the processing of larger components containing nanoscale materials
- Science based understanding of advanced synthesis and processing methods such as self-assembly, molecular-directed nanostructure formation, and novel deposition methods will be investigated. This understanding will be applied to attain new structures, to fabricate materials with new functionalities, and to reduce the energy and environmental impact of processing.
- Processing research will be extended to include new ceramic, intermetallic, semiconducting, organic and biomimetic materials and material structures, including nanocrystalline materials, films, coatings, and crystals. Analytical techniques and modeling will be developed and applied to determine and predict the relationship of synthesis and processing parameters to structure, purity, deformability, residual stresses, toughness, adhesion, and electronic, optical, and magnetic properties.
- The single crystal growth and bulk materials processing capabilities of the MPC will be updated and expanded to better serve the x-ray and neutron scattering communities

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Research Activity: Engineering Research

Division:	Materials Sciences and Engineering
Primary Contact(s):	Timothy Fitzsimmons (Tim.Fitzsimmons@science.doe.gov; 301-903-9830)
Team Leader:	Helen Kerch (Acting)
Division Director:	Harriet Kung

Portfolio Description:

Engineering Research advances scientific understanding underlying the dynamic interactions of single and multicomponent solid and fluid systems. Research considers the behavior and interactions of fluids including organic, biological, and complex fluids with each other and with solid systems; the transport of energy on and within these systems; and the development of means to advance the characterization of these systems. Issues under consideration frequently span several orders of magnitude in length and time scales and range from atomic interactions to macroscopic behavior and subpicosecond chemical events to fatigue events that may take years to reach completion. Accordingly they present a considerable challenge to theory, computational simulation, and experiment. Questions of interest have included understanding and predicting the behavior of (1) nanoscale structures and systems, including those with biological components; (2) dynamics of fluids, especially multi-component and complex fluids, but also including heat transfer, solidification, and granular materials; and (3) interactions of phonons with interfaces, secondary phases, or micro- and nanoscale defects in solids.

Unique Aspects:

The program is closely linked with the materials and chemical science activities of BES. Engineering Research has played a unique role in the National Nanotechnology Initiative (NNI) and Hydrogen Fuel Initiative (HFI) to further the understanding of nano- and meso-structures, devices and systems; molecular machines; transport behavior to and within consolidated nano-particulate material; and the dynamic behavior of multiphase, complex and biologically inspired materials, high surface area materials, consolidated nano-particulate materials, dispersion and coatings, photonics, nano-devices and molecular machines using nano-scale building blocks. This activity has had a leadership role in the fundamental understanding of multiphase fluid flow, heat transfer, and the fundamental behavior of granular materials.

Relationship to Other Programs:

Department of Energy (DOE)

- Office of Nuclear Energy Science and Technology (NE) - Nuclear Energy Research Initiative
- Office of Environmental Management (EM) - Environmental Management Science Program

Other Federal Agencies:

- National Science Foundation (NSF) – Exploring the possibilities of a joint initiative on neural electronics
- Interagency Working Group on Nanotechnology (NSTC/CT/MatTec)
- NSF, Department of Defense (DOD), and National Aeronautics and Space Administration (NASA) – Joint funding of research on Molecular Motor
- DOE representative on the Interagency Quantum Information Science Coordinating Group (NSTC/CT)
- Interactions with the community through: (1) workshops, such as the Workshop on Multiphase Fluid Flow, May 2002, and the Symposium on Computational Approaches to Disperse Multiphase Flows, October 2004; and (2) program presentations to the American Society of Mechanical Engineers, the American Society for Engineering Education, and other groups.

Significant Accomplishments:

- Assisted in creating an energy efficient chemical industry by developing databases, estimation techniques, and design models. ASPEN Tech was founded using these tools and now has over 1500 employees worldwide.

- Oil and gas companies are using results of research for more efficient transport and exploration of crude oil and natural gas. The Syncrude pipeline would not have been built without these developments that results in a 97% saving in energy used to transport the crude.
- Research on micro and nano systems has resulted in the developments of a nanosized biological motor for use in MEMS and NEMS devices
- Research on nanomotion from biomolecular interactions has led to the development of instruments for detecting and identifying molecules
- Adding small quantities of carbon nanotubes to a fluid dramatically increases its ability to conduct heat; however, theory predicts an even larger increase in conductivity. Experiments and simulations point to poor thermal coupling between the nanotubes and the fluid with implications for designing advanced heat transfer systems. Nanofluids have been created that conduct heat ten times faster than predicted possible.
- The thermal conductivity of single crystal silicon nanowires has been discovered to be two orders of magnitude lower than the bulk thermal conductivity of silicon. This is highly desirable property for thermoelectric applications. Simultaneously, the results reveal their limitation highly undesirable for many electronics and photonics applications.
- Record of heat flux dissipation has been achieved with a micro-channel two-phase flow (27,600 W/cm^2)

Mission Relevance:

New and improved understanding of dynamic behavior capabilities at the nano- and microscale will improve materials properties through improvements in processing and quality techniques, increased computing speed, improved sensing and control capabilities, further understanding leading to accurate predictions of materials and systems behavior, and enable larger-scale applications of devices with nano-scale components. Together these advances will further lead to higher process efficiency and lower energy consumption. Improving the knowledge base on multi-components fluid dynamics and heat transfer will have a major impact on energy consumption, because these phenomena are an integral part of every industrial process. Potential impacts include improved efficiency of fossil and nuclear based power generating systems.

Advances in non-linear dynamics will lead to improved control and predictive capabilities of complex systems, thus resulting in higher efficiency and lower energy consumption.

Scientific Challenges:

Focus areas include: accurate modeling of the transport of hydrogen and heat through nanoscale materials, and nanoporous and mesoporous structures; the understanding of anomalous thermal behavior of nanofluids and nanowires; understanding where continuum approximations break down in multicomponent systems containing fluids; describing, simulating, and engineering macroscale systems to take advantage of nanoscale behavior. Challenges also include understanding: (1) the potential of chemical and biological systems to construct complex, nanostructured materials under ambient conditions; (2) the role of interfaces and structure on the behavior of simple and complex fluids; (3) how more realistic sized groupings of drops and bubbles interact with each other and with their environment; (4) the mechanics and energetics of molecular mechanical devices, thus providing the foundations for their eventual use; (5) simple and complex systems driven far from thermodynamic equilibrium; and (6) the interactions of phonons with defects and interfaces.

Challenges in engineering sciences include identifying those scientific discoveries within the BES program that are most appropriate to pursue within the context of the energy and environmental mission needs of DOE, while supporting developments of engineering principles that enable scientific breakthroughs to be used for:

- Changing processes so that engineered systems are more energy efficient and environmentally friendly.
- Developing mathematical models of systems that can be used to make them better.
- Understanding the limitations of systems and extend those limits

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
5,306	2,444	1,000

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

Shifts in research priorities and corresponding decreases in budget mandate an orderly completion of ongoing activities.

Research Activity: Neutron and X-ray Scattering

Division:	Materials Sciences and Engineering
Primary Contact(s):	Helen M. Kerch (Helen.Kerch@science.doe.gov; 301-903-2346)
Team Leader:	Harriet Kung (Acting)
Division Director:	Harriet Kung

Portfolio Description:

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials as well as the relationship of these structures and excitations to the physical properties of materials. The continuing development and improvement of next-generation instrumentation including a full range of elastic, inelastic, and imaging techniques as well as ancillary technologies such as novel detectors, sample environment, data analysis, and technology for producing polarized neutrons is also supported.

Unique Aspects:

The Department of Energy (DOE) history and mission have played important roles in BES' current position as the nation's steward of major neutron and x-ray facilities. Historically, neutron sources descended from the nuclear reactors that were constructed in the early 1940s as part of the U.S. Atomic Energy Program. Similarly, synchrotron facilities stemmed from particle accelerators that were developed for high-energy physics research. As part of its stewardship responsibilities, BES maintains strong fundamental research programs in materials and related disciplines that are carried out at these facilities by the laboratory, university, and industrial communities. This activity has evolved from the pioneering, Nobel prize-winning efforts in materials science to the current program that encompasses multiple techniques and disciplines. The activity also supports the research that has motivated the largest BES construction projects in recent years - the Advanced Light Source (ALS), Advanced Photon Source (APS), and Spallation Neutron Source (SNS). BES is a major supporter of both the research and the instrumentation at these and other facilities. Neutron and x-ray scattering are well-established techniques for investigating the microscopic properties of materials. With the advent of both high brightness x-ray beams produced by third generation synchrotron radiation facilities and intense pulsed neutron beams provided by accelerator-based neutron sources, a number of totally new capabilities will become possible.

Neutron Scattering - Neutron scattering provides information on the positions, motions, and magnetic properties of solids. With unique characteristics such as sensitivity to light elements, neutron scattering has proven to be invaluable to polymer and biological sciences. The high penetrating ability of neutrons allows property measurements and nondestructive evaluation deep within a specimen. Neutrons have magnetic moments and are thus uniquely sensitive probes of magnetic species within a sample. The wavelength of neutrons used in scattering experiments is commensurate with interatomic distances, and their energy (meV) is comparable to both lattice and magnetic excitations (phonons and magnons) making them an ideal probe for both structure and dynamics.

X-ray Scattering - The unique properties of synchrotron radiation–high flux and brightness, tunability, polarizability, high spatial and temporal coherence, along with the pulsed nature of the beam–afford a wide variety of experimental techniques in diffraction and scattering, spectroscopy and spectrochemical analysis, imaging, and dynamics.

Relationship to Other Programs:

This activity interacts closely with research instrumentation programs supported at other federal agencies, especially in the funding of beam lines whose cost and complexity require multi-agency support. The activity works in concert with the Instrumentation for Materials Research – Major Instrumentation Projects (IMR-MIP) at the National Science Foundation (NSF) and the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) in the Department of Commerce to develop instruments and capabilities that best serve the national user facility needs. A coordinated effort between DOE and NSF is ongoing to facilitate the full use of the nation's neutron scattering facilities under the auspices of the Office of Science and Technology Policy Interagency Working Group on Neutron Science. In FY 2005, the program coordinated technical topics with the DOE Small Business Innovation Research (SBIR) Program which resulted in 6 Phase I and 2 Phase II awards in the area of neutron detectors, monochromators, and other scattering instrumentation.

Significant Accomplishments:

Neutron Scattering - This activity supported the research of Clifford G. Shull at Oak Ridge National Laboratory (ORNL) that resulted in the 1994 Nobel Prize in Physics for the development of the neutron diffraction technique. Shull's work launched the field of neutron scattering, which has proven to be one of the most important techniques for elucidating the structure and dynamics of solids and fluids. The program supports major efforts in neutron scattering centered primarily at the DOE national laboratories of Ames, Argonne, Brookhaven, Oak Ridge, and Los Alamos; these groups have pioneered virtually all the instruments and techniques in neutron scattering, spectroscopy, and imaging.

X-ray Scattering **-** As in the neutron scattering effort, the program supports large research groups that use synchrotron radiation to understand the intrinsic properties of materials. These groups have contributed to the development of such powerful techniques as magnetic x-ray scattering, inelastic x-ray scattering, extended x-ray absorption fine structure (EXAFS), x-ray microscopy, microbeam diffraction, time-resolved spectroscopy and others.

Recent accomplishments include the development of Kirkpatrick-Baez neutron focusing optics for spatially resolved neutron scattering; determination of spin structure interactions in exchange bias, lensless imaging of magnetic nanostructures by x-ray spectro-holography; the first measurements of the structure of ^{4}He adsorbed on carbon nanotubes; and elucidation of the role of phonons in colossal magnetoresistance.

Mission Relevance:

The increasing complexity of energy-relevant materials currently of interest to the Office of Energy Efficiency and Renewable Energy such as superconductors, semiconductors, and magnets requires ever more sophisticated scattering techniques to extract useful knowledge and to develop new theories for the behavior of these materials. X-ray and neutron scattering, together with the electron scattering probes supported under Structure and Composition of Materials, are the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. Additionally, neutrons will play a key role in the President's Hydrogen Fuel Initiative as they provide atomic- and molecular-level information on structure, hydrogen diffusion, and interatomic interactions, as well as the nanoscale and macroscopic morphologies that govern useful properties in catalysts, membranes, proton conductors, hydrogen storage materials, and other materials and processes related to hydrogen production, storage, and use. The program is relevant to National Nuclear Security Administration in its activity on the behavior of matter in extreme environments, especially high pressure. This is the Nation's largest program in neutron and x-ray scattering in condensed matter physics and materials physics supporting the science performed with scattering tools, and the concomitant development of techniques and instrumentation. Consequently it underpins the facility stewardship role of DOE by enabling full exploitation of the BES synchrotron light sources and neutron scattering facilities. The scattering program interfaces with other programs in BES, including: Theoretical Condensed Matter Physics in scattering theory and models; Materials Chemistry and Biomolecular Materials in scattering probes and techniques for soft matter and biophysical materials interrogation such as spin echo spectroscopy, neutron reflectometry, and grazing incidence small angle scattering; Geosciences Research in high pressure neutron and x-ray scattering techniques and tools; and Heavy Element Chemistry in molecular level and surface actinide speciation information.

Scientific Challenges:

Correlated Electron Systems - The effects of strong electron-electron interactions give rise to a remarkable range of anomalous behavior in condensed matter systems, producing phenomena as varied as metal-insulator transitions, colossal magnetoresistance, and high temperature superconductivity in heavy fermion metals, insulators, and magnets. In particular, high-temperature superconductivity is a singularly spectacular example of the cooperative macroscopic phenomena such as the interplay of charge, spin, and lattice degrees of freedom that can arise from correlated electron behavior. Techniques such as inelastic x-ray scattering and neutron diffraction, among others, have enabled scientists to unravel the crystallographic and microscopic electronic structure of these materials, including stripes. This information will ultimately be used to answer questions such as what is the mechanism for superconductivity, how high can the temperature be for materials to remain superconducting, and will that temperature ever be room temperature.

Matter Under Extreme Conditions - Opportunities in high pressure research address a broad range of new scientific problems involving matter compressed to multimegabar pressures. Extreme pressures provide a fertile ground for the formation of new materials and novel physical phenomena as compression changes the chemical bonds and affinities of otherwise familiar elements and compounds. Highly collimated and intense synchrotron beams provide the ideal source for ultrafine and sensitive x-ray diffraction microprobes necessary to measure concentrated high stresses in a very small area. With the development of the SNS, innovative focusing optics, more sensitive detectors and emerging next-generation pressure cells, high pressure research at neutron sources can approach the routine pressure ranges available with diamond anvil cells at synchrotron x-ray sources. With the dramatic advances in techniques for preparing and investigating single crystals, studies of more complex materials become tractable. Similarly, scattering experiment performed in the presence of magnetic fields can be used to study materials during phase transitions (magnetic, structural, and superconducting) thus allowing researchers to segregate magnetic field effects or to simulate effects normally observed via doping (for example).

In-situ Studies of Complex Materials - Recent advances in both sources and instrumentation have yielded gains in intensity on sample facilitating rapid experiments and in-situ configurations. Smaller samples can be probed with unprecedented resolution, accuracy, and sensitivity under various parametric conditions. In-situ synchrotron radiation techniques provide real-time observations of atomic arrangements with high spatial sensitivity and precision, which are important features in the development of novel processing techniques and in the search for new exotic materials. In-situ studies of complex materials including those undergoing time-dependent structural or magnetic phase transformations, disordered systems such as alloys and amorphous materials, organic thin films and self-assembled systems, and other condensed matter systems can be probed with a variety of scattering, reflectivity and spectroscopic techniques.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
46,061	45,141	62,055

Performer	Funding Percentage
DOE Laboratories	76%
Universities	24%

Major DOE national laboratory performers include Ames, Argonne, Brookhaven, Oak Ridge, Los Alamos, and the Stanford Linear Accelerator Center.

This activity also provides support for the construction of seven instruments at the SNS including; High-Resolution Chopper Spectrometer (ARCS); Cold Neutron Chopper Spectrometer (CNCS); Ultra High Pressure Diffractometer (SNAP); High Resolution Thermal Chopper Spectrometer (SEQUOIA); Single Crystal Diffractometer (SCD); Disorder Materials Diffractometer (NOMAD); and the Hybrid Spectrometer (HYSPEC). Also supported is the operation of MUCAT (Midwest Universities Collaborative Access Team) and HPCAT (High Pressure Collaborative Access Team). Funding at the Stanford Linear Accelerator Center includes support for the Ultrafast Science Center.

Projected Evolution:

Advances in neutron and x-ray scattering will continue to be driven by the scientific opportunities presented by improved source performance and instrumentation optimized to take advantage of that performance. The x-ray and neutron scattering activity will continue in fully developing the capabilities at the DOE facilities by providing instrumentation and research support. A continuing theme in the scattering program will be the integration and support of materials preparation (especially single crystals) as this is a core competency that is vital to national interests.

Neutron Scattering - The ongoing enhancements at the High Flux Isotope Reactor (HFIR) will not only increase the nation's neutron scattering capacity, but, in many cases, will provide instruments with resolution and flux on sample that is equal to or greater than existing benchmark instruments. The Spallation Neutron Source (SNS) will push instrument capacity and performance even further. One challenge for this activity will be to support an increased research effort in neutron scattering to take full advantage of the improved sources and to prepare for the SNS. Another includes maintaining the strength of the DOE national laboratory-based neutron scattering groups and rebuilding strength in neutron sciences in the academic community. Education and training of the next generation of neutron scientists – especially those familiar with instrumentation and performance of TOF methods – remains a high priority.

X-ray scattering - Major instruments at the synchrotron light sources have a lifetime of 7-10 years. Thus a challenge to the program is to provide support for the 10-15% of the instruments which must be upgraded or replaced each year to keep the facility at the forefront of science.

Research Activity: Experimental Condensed Matter Physics

Division: Materials Sciences and Engineering
Primary Contact(s): James Horwitz (james.horwitz@science.doe.gov, 301-903-4894)
Team Leader: Harriet Kung (Acting)
Division Director: Harriet Kung

Portfolio Description:

This program supports activities in experimental condensed matter physics that emphasize the relationship between electronic structure and the properties of complex systems whose behavior is often derived from electron correlation. Major efforts are in systems that exhibit correlated and emergent behavior with superconducting, semiconducting, magnetic, thermoelectric, and optical properties. These efforts are accompanied by activities to synthesize and characterize single crystals to further explore and discover new and novel correlated electron behavior. The program supports the development of new techniques and instruments for characterizing the properties of these materials under extreme conditions of ultra low temperature (mK) and ultra high magnetic fields (100 T). One main emphasis of this activity is on the electron dynamics of low dimensional systems. Confinement effects in high purity semiconductors produce new forms of matter and new physical phenomena such as the fractional Quantum Hall effect and Bose-Einstein Condensates. These low dimensional systems and other nanophase materials offer rich opportunities to explore their novel electronic behaviors. In addition, this activity seeks to exploit ultrafast tools to manipulate and probe the dynamic electronic behavior of condensed matter through the development and applications of laser-driven, table-top x-ray sources.

Unique Aspects:

The research on magnetism and magnetic materials has more emphasis and direction than in other federally supported programs. It focuses on hard magnet materials, such as those used for permanent magnets and in motors, and on exchange biasing, such as used to stabilize the magnetic read heads of disk drives and the influence of nm length scales on magnetic materials properties. The Experimental Condensed Matter Physics (ECMP) activity continues to support research on electronically complex materials, an area that impacts a wide range of other topics including superconductivity, magnetoresistivity, low-dimensional electron systems, and magnetism including topics such as exchange bias and spin-polarized electron transport. The combined projects in superconductivity comprise a concerted and comprehensive energy-related basic research program. The Department of Energy (DOE) national laboratories anchor the efforts and maintain the integration with the Office of Electricity Delivery and Energy Reliability (OE) developmental efforts. The 100 T multi-shot magnet, under construction at the Los Alamos National Laboratory (LANL), is a multidisciplinary project in many different areas of materials design, materials research, and high power systems. Two major areas research will be pursued upon completion of the magnet in 2006 which include magnetic field induced phase transitions in addition to nano-quantization and quantum size effect. The ECMP activity also has unique thrusts in photoemission investigations of cuprate superconductors. It is a source of new materials scientists through strong programs at LANL, Sandia National Laboratories (SNL), Ames Laboratory, Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), and the Stanford Linear Accelerator Center (SLAC)**.** Internationally, the ECMP activity holds a position of world leadership in the areas of magnetism, superconductivity, materials characterization, and nanoscale science. New, exciting areas launched within this activity in photonic band gap materials, 2-D electron systems, magnetic superconductors and quasicrystals are now pursued worldwide. Enhanced efforts are ongoing to generate high quality single crystals of new materials at Ames, ANL, BNL, Oak Ridge National Laboratory (ORNL), and SLAC.

Relationship to Other Programs:

This activity supports the National Academy of Science's Solid State Sciences Committee, which in turn serves as a coordinating mechanism nationally. It also supports topical activities at the National Academy of Sciences which include the *Decadal Assessment and Outlook for the Field of Condensed Matter and Materials Physics (CMMP) Research* and *An Assessment of New Materials Synthesis and Crystal Growth in the United States*. This research in the ECMP program is aimed at a fundamental understanding of the electronic behavior of materials that underpin DOE technologies. Improving the understanding of the physics of materials on the nanoscale will be technologically significant as these structures offer enhanced properties and could lead to dramatic improvements in energy generation, delivery, utilization, and conversion technologies. Specifically, research efforts in understanding the fundamental mechanisms in superconductivity, the elementary energy conversion steps in photovoltaics, and the energetics of hydrogen storage provide the major scientific underpinnings for the energy technologies. The granular materials research contributes to our understanding of radionuclide transport in groundwater and is of direct relevance to the environmental clean-up efforts. This activity also supports research of fundamental interest for information technology and electronics industries in the fields of semiconductor and spintronics research. These research efforts are closely coordinated with other core research activities in BES, including the Physical Behavior of Materials on photovoltaics, Synthesis and Processing Science on single crystal growth, X-ray and Neutron Scattering on photoemission studies, and Theoretical Condensed Matter Physics on nanostructures and low-dimensional systems. They are also coordinated with DOE technology programs in the Office of Energy Efficiency and Renewable Energy (EERE), OE, and Office of Environmental Management (EM).

Significant Accomplishments:

The ECMP activity has a long history of accomplishments dating back to the 1950s and the first neutron scattering experiments at ORNL. Notable accomplishments include the discovery of ion channeling and the development of the field of ion implantation; the discovery of metallic and strained-layer superlattices; the establishment of the field of thermoacoustics and thermoacoustic refrigeration and heating; the invention of Z-contrast scanning transmission electron microscopy; the theoretical and predictive basis for photonic band gap materials; the tandem photovoltaic cell; the observation of stripes in superconductors, the invention of a Josephson junction scanning tunneling microscope and the first observation of superconductivity in a magnetically doped semiconductor ($PtSb_2$ with ~1% Yb), the observation of Bose condensation of excitons doped double layer semiconductor structures, and the characterization of BCS and 2 Gap Superconductivity in magnesium diboride (MgB_2). In addition, the activity has supported much of the seminal work in the fields of high temperature superconductors and quasicrystals, efforts now pursued worldwide.

Mission Relevance:

This activity provides direct research assistance to the technology program in OE on superconductivity. In addition, it supports, more fundamentally, several DOE technologies and the strategically important information technology and electronics industries through its results in the fields of semiconductor physics and electronics research; the petroleum recovery efforts of the Office of Fossil Energy (FE); and the clean-up efforts of EM through research on granular materials and on fluids; and the R&D on advanced materials and magnets and thermoelectrics of EERE.

Scientific Challenges:

Among the immediate on-going scientific challenges are: the solution of the mechanism for high temperature superconductivity; the understanding of “stripes” in correlated electron systems; the understanding of novel quantum effects and of “emergent phenomena,” that is, new phenomena that emerge when the complexity of a system grows with the addition of more particles; the development of a very high-magnetic field research program to exploit the 100T and 60T magnets at LANL; research in nanoscale science; low-temperature physics; and the continued development of a materials synthesis and crystal growth capability in this country. Quality materials lie at the heart of quality measurements: a thrust to develop a core competence in the synthesis of new materials and the growth of crystals is underway, and it will continue to be a priority. High-magnetic-field research coupled with low temperature physics led to the discovery of the quantum Hall effect and to the general area of novel quantum effects. The availability of very high magnetic fields over useable time scales, as will be afforded by the new magnets at LANL, offers the promise of both increasing the fundamental understanding of matter and of observing the effects of very high magnetic fields on materials properties. This will undoubtedly lead to the discovery of new and exciting physics. Similarly, low temperature physics continues to be important for the advancement of physics by providing the experimental conditions necessary to observe phenomena such as BEC, the quantum Hall effect, and superconductivity. Developing and understanding matter and materials at the nano- and subnanoscale is a critical need because electronic, optical, and magnetic devices continue to shrink in size. Ballistic transport in quantum wires exceeding 5 μm in length may provide the basis for quantum computing.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
41,024	36,691	47,480

Performer	Funding Percentage
DOE Laboratories	77%
Universities	23%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

The Experimental Condensed Matter Physics activity will include further work at the nanoscale; the development of a very high magnetic field research program; and continued development of the materials synthesis and crystal growth thrust. The portfolio can be expected to continue thrusts in electronic structure, new materials, surfaces/ interfaces, and experimental techniques. For example, sum frequency generation is a new technique that is now being used to probe the electronic and vibrational structure of chiral molecules on surfaces. Femtosecond time-resolved magnetooptical, tehahertz and x-ray diffraction techniques will be used to study the coupled dynamics of charge carriers along with the associated lattice deformations in high temperature superconductors, colossal magneto-resistance manganites and charge density wave conductors. The subtopics also will be the similar, e.g., magnetism, low dimensional electron systems, and new materials. Low temperature physics and superconductivity are important. Low temperature physics underlies several other areas of opportunity and presents issues of its own. Superconductivity, specifically high temperature superconductivity, continues to be a potentially revolutionizing technology. The goal for the former is to augment the investment in low temperature physics when possible. In superconductivity, the goal is to identify the most pressing scientific issues and ensure the level of effort is consistent with the priorities. New investigations in the Casimir force have been initiated. This attractive force between two surfaces in a vacuum predicted over 50 years ago could affect everything from micromachines to unified theories of nature.

Research Activity: **Condensed Matter Theory**
Division: Materials Sciences and Engineering
Primary Contact(s): Dale Koelling (Dale.Koelling@science.doe.gov , 301-903-2187)
Team Leader: Harriet Kung (Acting)
Division Director: Harriet Kung

Portfolio Description:

The Condensed Matter Theory activity supports basic research in theory, modeling, and simulations complementing the experimental effort. A current major thrust is in nanoscale science where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other research areas include correlated behavior of two dimensional electron gases, quantum transport, superconductivity, magnetism, and optics. An important facilitating component is the Computational Materials Science Network (CMSN) which enables groups of scientists from Department of Energy (DOE) national laboratories, universities, and (to a lesser extent) industry to address materials problems requiring larger-scale collaboration across disciplinary and organizational boundaries.

Unique Aspects:

New areas of materials science are being identified and studied. New technology is enabling a much closer examination of the existing ones. This healthy progress dictates that new theories be developed and that established ones be reexamined and possibly extended. A very important contribution of the theorist is enforcing a rational, consistent understanding of experimental observations so that we can go forward. Often, this involves working out implications of a theory for a specific material or situation. In materials, this can be an extremely difficult task owing to the very many atoms involved. Theorists have developed many conceptual tools such as quasiparticles, entities defined to examine phenomena at different length scales, or summary statistical approaches to deal with this problem. Further development of such conceptual tools continues to be a very important aspect within this theoretical program. However, for many phenomena now being studied, large scale computation must be used to perform the complex calculations dictated by the fundamental theory or to perform the simulations of systems with many interacting components. The rapid advance in computational capabilities now enables research at such a level of sophistication that computational science has become a “third way of doing science,” albeit, at a price. The complexity of such research often dictates larger groups of collaborating researchers from a diversity of disciplines and one response is CMSN. At present, CMSN consists of six sub-projects: Excited States and Response Functions (testing the accuracy of current levels of fundamental theory); Microstructural Effects on the Mechanics of Materials (computational study of the fundamental basics of metallurgy); Fundamentals of Dirty Interfaces: From Atoms to Alloy Microstructures (the development of microstructure in heterogeneous materials); Magnetic Materials Bridging Basic and Applied Science (an attempt to interconnect different scales of magnetic behavior from quantum mechanical electronic behavior all the way to continuum micro-mechanical properties); Predictive Capability for Strongly Correlated Systems (an attempt to advance capabilities in many body theory); and Multiscale Studies of the Formation and Stability of Surface-Based Nanostructures.

Relationship to Other Programs:

This activity interacts with all the other research activities within the BES Materials Science and Engineering Division, driven by mutual interest. Because production supercomputer resources used by the division are administered in this activity, there is an enhanced awareness of opportunity. Within the Office of Science, frequent interaction occurs with the Mathematical, Information, and Computational Sciences Division. Information on university grants is shared with the National Science Foundation (NSF), peer reviews are sometimes shared, and on occasion there is joint funding of grants. On the international level participation in organizing and steering committees is frequent, as are exchanges of experts between foreign and domestic institutions.

Significant Accomplishments:

Consistent with an emphasis on nanoscience, notable achievements in this area have been made within this activity. Research into low dimensional materials has revealed exciting new information and has pointed to new possibilities in creating new tailored materials and devices. Highlights include:

- By judiciously attaching molecules to nanoclusters, one can guide them to assemble in a specified manner. (The rule book remains to be written, but it is under construction.)

- Gold nanoparticles behave much more like their platinum group neighbors in the periodic table including exhibiting interesting catalytic behavior. When passivated by dodecane thiols, they can self-assemble into nanocrystalline superlattices with unique properties.
- Nanocrystalline diamond can form with a bucky ball-like surface reconstruction. The carbon nanoparticles exhibit very weak quantum confinement unlike silicon and germanium.
- Silicon nanotubes can be formed by stabilization with a core of nickel atoms. Unlike carbon, silicon nanotubes are not stable without such help.

Significant progress has also been made in other areas as illustrated by the following examples:

- Dynamic mean-field theory, which is exact for infinite dimensions, has been successfully coupled with three dimensional band theory. The resulting hybrid theory has been used to elucidate the spin polarization of CrO_2– a famous magnetic recording material that might find new use in spintronics. A competition between quasiparticle behavior and local-moment behavior is found.
- Progress has been made on the question of how to treat core-hole effects in x-ray absorption spectra by a collaboratory research team of the CMSN. The team, which focuses on Excited States and Response Functions, brought together experts of all applicable approaches to compare approaches and elucidate the formal relationships among them. What resulted was an excellent prescription for success but with identified places for improvement. This is needed not only for fundamental understanding of the details of x-ray absorption phenomena but for technological applications, e.g. the measurement of the thickness of integrated circuit interconnects.
- The origin of the light-induced conductivity in the transparent oxide $12CaO{\cdot}7Al_2O_3$ is traced to electrons excited off hydrogen H ions present. To accomplish this, it was first necessary to accomplish calculating the Coulomb gap leading to hopping conductivity.
- A way has been found to see diffraction data for molecules adsorbed on surfaces. The conventional methods of low energy electron diffraction will not work; the molecules produce no Bragg spots because they are randomly distributed on the surface. However, it has been shown that the information is present in the intensity variation of the spots originating from the substrate. The resulting technique has successfully revealed the geometry of small hydrocarbons on a palladium surface.

Mission Relevance:

The program's ultimate purpose is to understand the properties of existing materials and to reveal new ones that are more efficient in producing, storing, and using energy. To this end, the programs in this portfolio have the common goal of achieving a basic understanding of matter at all scales ranging from atomic to bulk. The experimental and theoretical programs work closely together, but there are also more independent modes of research. The theorists try to establish a theoretical basis for experimentally observed results, which almost always suggests further experiments, and thus leads to new results. New experiments and experimental techniques are suggested. New science is also produced by simulating processes on computers. "Computer experiments" can be performed which are difficult or impossible to perform in the laboratory. They are also much easier to dissect and to vary the conditions in order to isolate the effective mechanisms. For example, the behavior of the surface layers of materials sliding on each other and a new understanding of the role of lubricants has been obtained in this way. Other examples include investigations into the behavior of electrons flowing in nano wires and nanotubes and in the properties of matter at extreme conditions of temperature and pressure.

Scientific Challenges:

The close relationship between the experimental and theoretical programs dictates that many challenges are common to both. Examples are exploring the behavior of complex systems, investigating nano-scale systems, and understanding superconductivity. New ways of conceptually visualizing and characterizing phenomena will broaden our horizons. Stripes occurring in cuprate superconductors and two dimensional electron gasses are excellent examples. Bridging length scales is a major thrust. The tactic of dividing up the effects in materials according to the length scale at which they occur has greatly facilitated our understanding. But for theorists, this creates the problem of how to pass needed information between the different constructs used at the different length scales. Only in that way can one calculate parameters rather than make phenomenological fits. Such is the basis for improved understanding and greater precision of our modeling. It is a continuing major goal on which limited progress has been made. Bridging time scales is similarly important, but far less progress has been made. Basic theory improvements are also needed. For example, density functional theory is our most computationally tractable many body theory, but it defines many functionals both for the ground state or ensemble energy and separately for the properties that must be determined. Whereas knowledge of the exchange-correlation functional for the ground state energy is reasonably advanced, knowledge of all other functionals is still quite rudimentary. Other many body approaches, although far more computationally intensive, provide important information and require further development. Improvements are also needed in our computational tools. Materials theory is a very heavy consumer of computer resources even if not so visibly as other disciplines. (This is because materials theory deals with many dissimilar problems rather than a few overarching ones.) The materials community could make very productive use of vast increases in computational capability. Because the phenomenal growth due to hardware improvements is actually overshadowed by those due to clever algorithm design, further improvements in "tool development" will significantly impact future development of science in a qualitative way.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
19,798	22,888	27,408

Performer	Funding Percentage
DOE Laboratories	56%
Universities	44%

The program provides funding for 65 university grants supporting about as many students and partially supporting about 64 faculty and senior staff. There are approximately 70 postdoctoral associates fully or partially supported by this activity. The program supports research at Lawrence Berkeley National Laboratory, Brookhaven National Laboratory, Ames Laboratory, Argonne National Laboratory, Oak Ridge National Laboratory, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and National Renewable Energy Laboratory. Programs at the national laboratories are multi-investigator efforts on problems that require extensive participation by experimental and theoretical scientists. Many of the research efforts at national laboratories involve interfaces with the university and industrial communities and with user facilities. Additionally, about $1.68M is provided for projects of the CMSN.

Projected Evolution:

Materials will be modeled with ever-greater sophistication, realism, and complexity. Needs and opportunities will drive the effort inexorably in this direction. Science at the nanoscale will continue a major thrust, although it is only one of many. A cooperative effort between the BES Chemical Sciences, Geosciences, and Biosciences Division and the Mathematical, Information, and Computational Sciences Division seeks to enhance our capabilities to model and simulate at the nanoscale. The CMSN will be enhanced to bring together teams adequate to address the more complex problems envisioned. Large scale computing will continue to be an important aspect of the research, but a new balance will have to be achieved in the allocation of resources, which will impact all BES activities.

Research Activity:	**Materials Chemistry**
Division:	Materials Sciences and Engineering
Primary Contacts:	Richard D. Kelley (Richard.Kelley@science.doe.gov; 301-903-6051) Aravinda M. Kini (Aravinda.Kini@science.doe.gov; 301-903-3565)
Team Leader:	Harriet Kung (Acting)
Division Director:	Harriet Kung

Portfolio Description:

This activity supports basic research in the design and synthesis of novel materials and material constructs with an emphasis on the chemistry and chemical control of structure and collective properties. Major thrust areas include: (1) nanoscale chemical synthesis and assembly–synthesis of nanoscale materials, manipulation of their properties, and organization of nanoscale materials into macroscopic structures; (2) solid state chemistry–exploratory synthesis and discovery of new classes of electrical conductors and superconductors, magnets, thermoelectric and ferroelectric materials, and porous materials with controlled porosities and tailored reactivities; (3) polymers–exploring and exploiting the self-assembly of block copolymers, polymer composites, and polymers with novel electronic and optical properties; (4) surface and interfacial chemistry–electrochemistry, electro-catalysis, friction, adhesion and lubrication at the nanoscale, and development of new, science-driven, laboratory-based analytical tools and techniques; and (5) biomolecular materials–biomimetic/bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology.

Unique Aspects:

Basic research supported in this activity underpins many energy-related technological areas. Focus of this activity on exploratory chemical synthesis and discovery of new materials is complementary to the emphasis on bulk synthesis, crystal growth, and thin films in the Synthesis and Processing Science activity. Similarly, the Biomolecular Materials activity with a focus on innovative materials complements the Energy Biosciences research, whose focus is on the chemical aspects of biomolecular systems. Significant interactions and collaborations exist between the principal investigators in this activity and the X-Ray and Neutron Scattering activity for the characterization of new materials by use of advanced scattering/spectroscopic tools at BES supported synchrotron and neutron facilities. Many of the scientists performing nanoscience-related work sponsored by this activity are also leaders of science thrust areas at the BES Nanoscale Science Research Centers.

A sizeable portion of the scientific thrusts pursued in this portfolio are multi-investigator and multi-disciplinary in nature. Investigators supported in this program are world leaders in solid state NMR and MRI, neutron reflectivity of soft matter, organic magnets, organic conductors and superconductors, biomolecular materials, polymer interfaces, nanoscience, organic-inorganic composite materials, basic science of tribology, and advanced inorganic materials including quasicrystals. Several investigators in this program are pioneers of novel instrumentation/ techniques such as high resolution MRI outside the magnet (Pines/Lawrence Berkeley National Laboratory, neutron reflectometers (Felcher/Argonne National Laboratory and Russell/University of Massachusetts), combinatorial materials chemistry for new materials discovery (Schultz/Scripps Research Institute), the surface force apparatus (Israelachvili/UC Santa Barbara and Steve Granick/University of Illinois, Urbana-Champaign), and spin-polarized metastable helium scattering (El-Batanouny/Boston University). The program has sought to identify and support high-risk, high-impact and often ground-breaking research, and will continue to do so.

Relationship to Other Programs:

The Materials Chemistry program is a vital component of the materials sciences that interfaces chemistry, physics, biology, and engineering. This interfacing results in very active relationships.

- Within BES, there are jointly funded programs in the DOE national laboratories and universities (about 10 currently), joint program reviews, joint contractor meetings, and programmatic workshops.
- Within DOE, there is coordination through the Energy Materials Coordinating Committee (EMaCC) which involves representatives of the Offices of Science (SC), National Nuclear Security Administration (NNSA), Fossil Energy (FE), Environmental Management (EM), Nuclear Energy Science and Technology (NE), Energy Efficiency and Renewable Energy (EERE), and Electricity Delivery and Energy Reliability (OE).
- Programs principal investigators are collocated and occasionally co-funded by EERE (batteries and fuel cells, green chemistry, solar energy conversion, and hydrogen storage), FE (catalysis and advanced materials research), and NNSA-Defense Programs (nanoscience research).

- Within the federal agencies, the program coordinates through the Federal Interagency Chemistry Representatives (FICR) which meets annually; the Interagency Power Working Group, which meets annually to coordinate all federal electrochemical technology (e.g., battery and fuel cell R&D) activity; the Interagency Polymer Working Group; and the NanoScience, Engineering, and Technology committee (NSET), which formulated the National Nanotechnology Initiative (NNI) and is currently a sub-committee of the National Science and Technology Council. This last committee meets monthly to coordinate the NNI.
- Very active interactions with the National Science Foundation (NSF) and National Institutes of Health (NIH) through joint workshops and joint funding of select activities as appropriate (two currently active).

Significant Accomplishments:

This program is responsible for pioneering the combinatorial materials chemistry approach for the discovery of new materials (Schultz, 1995). It is also responsible for the discovery of the first organic magnet (Miller and Epstein, 1986), the highest-T_c organic superconductor (Williams et al. 1990), the first all-organic superconductor (Williams et al. 1996), and the first room temperature organic magnet (Miller and Epstein, 1991). The latter discovery created a new field of research, which has grown substantially since then, and has transformed organic magnets from a scientific curiosity to a thriving scientific activity and is expected to have a huge impact on spintronics-based technologies. Recently, the first material that simultaneously exhibits bistability in three physical channels – electronic, magnetic and optical – was discovered (Haddon, 2002). A new approach involving the use of ordered intermetallic materials as fuel cell electrodes has been developed and offers great promise for finding a non-platinum, direct fuel cell that uses organic liquids (e.g., methanol and ethanol) as fuel (DiSalvo and Arbuna, 2003). A biomolecular route found in nature has been harnessed to produce a wide variety of photovoltaic and semiconductor nanocrystals at low temperature and under environmentally benign conditions (Morse, 2003, 2005). A truly remarkable recent achievement is the generation of a bacterium with a 21 amino acid genetic code, which can eventually lead to our ability to generate entirely new functional materials (Schultz, 2003, 2004, 2005). It will also be possible to extend this technology beyond proteins to prepare the long sought after monodisperse versions of industrial polymers such as polyesters and polyimides.

The program also pioneered the development of several cutting-edge techniques for probing materials, e.g., neutron reflectivity for the study of interfaces, buried interfaces, and interfacial phenomena in magnetic materials, polymers, colloids, biomaterials, and other complex, multicomponent materials. Every neutron scattering facility in the world now has neutron reflectometers, which are in great demand. The program pioneered and developed the use of laser polarized xenon to significantly enhance NMR spectra and MRI images, which has revolutionized medical diagnostics technology. Ex-situ NMR or NMR without magnets is another technique developed in this program, which is expected to have an enormous impact on imaging in materials science, biology and medicine, and airport screening (humans and baggage) technologies.

Mission Relevance:

The research in this portfolio underpins many energy-related technological areas such as batteries and fuel cells, catalysis, energy conversion and storage, friction and lubrication, high-efficiency electronic devices, hydrogen generation and storage, light-emitting materials, light-weight high-strength materials, and membranes for advanced separations. Materials Chemistry and Biomolecular Materials program provides support for fundamental research in surface and interfacial chemistry, nanoscience, polymeric and organic materials, solid state chemistry, and development of new tools and techniques to advance the field of materials sciences. Research in these areas is at the forefront of the synthesis, assembly, and understanding of materials.

Scientific Challenges:

The major challenge in this core research activity is identifying and supporting the research focused on exploratory synthesis and discovery of new materials with novel properties that can lead to entirely new energy-related technologies. Developing experimental strategies for the “atom-by-atom” synthesis of materials with unprecedented nanoscale (and sub-nanoscale) structural control is clearly an outstanding challenge. In this context, a detailed understanding of hierarchical and dynamic self-assembly processes ubiquitous in nature can be an extremely valuable guide. Such a knowledge base can lead to low-temperature, energy-efficient synthesis routes to new materials and new manufacturing processes.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007
46,860	40,694	49,748

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Performers (FY2005)	Funding Percentage
DOE Laboratories	63%
Universities	35%
Other	2%

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

In addition to maintaining a healthy core research activity, the program will further expand into nanoscience research, particularly at the nano-bio interface. It will seek to develop new multi-disciplinary approaches, with biology, chemistry, physics and computational science playing major roles, to model, design and synthesize new and novel materials. Some of the targeted areas that will receive support in the coming years include novel materials and innovative concepts that will impact solid state lighting, hydrogen production and storage, novel electrodes and membranes for improving the efficiency of fuel cells, and theory and modeling to aid new materials discovery. Also of particular interest is the development of new organic electronic materials with novel magnetic, conducting, and optical properties. The program will also facilitate multi-investigator, multi-disciplinary team research, to bring appropriate talents to bear on increasingly more complex and multi-functional materials. The program will continue to identify and support high-risk, high-impact, and often ground-breaking research.

Research Activity: Experimental Program to Stimulate Competitive Research (EPSCoR)

Division: Materials Sciences and Engineering
Primary Contact: Aravinda M. Kini (Aravinda.Kini@science.doe.gov; 301-903-3565) (Acting)
Team Leader: Harriet Kung (Acting)
Division Director: Harriet Kung

Portfolio Description:

The Department of Energy (DOE) Experimental Program to Stimulate Competitive Research (EPSCoR) activity supports basic research spanning the broad range of science and technology programs within DOE in states that have historically received relatively less federal research funding. EPSCoR includes the states of Alabama, Alaska, Arkansas, Delaware, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Tennessee, Vermont, West Virginia, and Wyoming, as well as the Commonwealth of Puerto Rico and the U.S. Virgin Islands. The work supported by EPSCoR includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, computational sciences, fossil energy sciences, and energy efficiency and renewable energy sciences.

Unique Aspects:

The program objective is accomplished by sponsoring two types of grants: (1) Implementation Grants, and (2) Laboratory-State Partnership Grants. Implementation grants are for a maximum period of six years with an initial grant period of three years. Maximum funding for these grants is $750,000 per year. Fifty percent state matching funds are required. The Laboratory-State partnership grants are for a period of one to three years. Maximum funding for these grants is $150,000 per year. Ten percent state matching funds are required. EPSCoR has placed a high priority on integrating the scientific manpower development component with the research component of the program. In addition, it is promoting strong research collaboration and training of students at the DOE national laboratories where unique and world-class facilities are available. This program is science-driven and supports the most meritorious proposals based on peer and merit review. Workshops and discussions are regularly held with representative scientists from EPSCoR states to acquaint them with the facilities and personnel at the national laboratories.

Relationship to Other Programs:

The activity interfaces with all other research activities within BES. In addition, it is responsive to programmatic needs of other program offices within DOE. The principal objective of the DOE EPSCoR program is to enhance the abilities of the designated states to conduct nationally competitive energy-related research and to develop science and engineering manpower to meet current and future needs in energy related areas. Most of the research clusters that have graduated from the DOE EPSCoR program after six years of funding have found alternate funding for continuing the research activity. This demonstrates that the research clusters funded by EPSCoR are becoming competitive. In addition, EPSCoR grants are supporting graduate students, undergraduates, and postdoctoral associates, and encouraging them to be trained in frontier research areas by making use of world-class research facilities at the national laboratories. The work supported by the EPSCoR program impacts all DOE mission areas including research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, advanced computer sciences, fossil energy sciences, and energy efficiency and renewable energy sciences.

Significant Accomplishments:

The EPSCoR program funds basic research in support of all programmatic needs of DOE. The accomplishments are grouped according to the relevant DOE program office.

Basic Energy Sciences

- Neutron Scattering of Thin Films and Interfaces: Neutron scattering is undergoing a revolution due to vast improvements in sensitivity and resolution made possible with upgrades at the High Flux Isotope Reactor (HFIR) and the construction of the Spallation Neutron Source (SNS). Neutrons make it possible to make unique measurements of magnetic materials which are inaccessible with other techniques. Magnetic materials are currently used in the information storage industry for hard drives and in the near future for nonvolatile magnetic random access memories. Neutron scattering techniques are necessary for understanding the fundamental properties of the materials. To improve these techniques a neutron analyzer with horizontal focusing was developed at the University of Alabama.

- This focusing analyzer is being implemented in a neutron spectrometer at HFIR. The spin structure of antiferromagnetic films and oxide materials was studied with neutron scattering techniques. Improvements in sample fabrication and characterization techniques are resulting in a more comprehensive understanding of the relationship between structure and magnetism in epitaxial antiferromagnetic films. This type of fundamental materials science research should aid in increasing the storage density, miniaturizing storage units, increasing data rates, and reducing the cost per bit in storage devices (Gary Mankey, University of Alabama).
- Enhanced Chemical Ordering in Ilmenite-Hematite Magnetic Semiconductors: This study demonstrated the enhancement of the magnetic moments of $FeTiO_3(1-x)/Fe_2O_3(x)$ semiconductor ceramic samples through irradiation with 40 MeV protons. The magnetic moment is directly related to the chemical order in the crystal structure. Thus, it is inferred that the proton irradiation reduces defects in these semiconductor ceramics. This effect allows for production of high-moment magnetic semiconductors for spin electronic applications. Moreover, this technique could lead to improved material properties in other systems, such as composite materials with thermally sensitive components like organic layers or metallic multilayers (R. K. Pandey, University of Alabama).
- Carbon nanotube-supported nanoparticle catalysts: Nanometer-sized metal particles are extremely active chemically because of their high surface-to-volume ratios. Scientists at the University of Idaho have developed methods of depositing and stabilizing nanometer-sized platinum group metals on surfaces of carbon nanotubes in supercritical fluid carbon dioxide. Uniformly distributed monometallic and bimetallic nanoparticles with narrow size distributions are formed on surfaces of carbon nanotubes using this method. The carbon nanotube-supported palladium (Pd) and rhodium (Rh) nanoparticles are far more effective than commercial carbon-based Pd and Rh catalysts for hydrogenation of olefins and aromatic compounds. These new nanoscale catalysts are currently being tested as electrocatalysts for low temperature polymer electrode fuel cells applications.

Biological and Environmental Research

Structural Biology and Computational Biology: The ability of an individual to form a clot primarily depends on the generation of a protein called thrombin. The process is aided by another protein called factor Va. Faculty and students at the University of Vermont have recently solved the 3-dimensional structure of bovine factor Va_i, a fragment of factor Va, which provides an essential look at how this protein may function to regulate thrombin production. Due to its similarity to factor VIII, one of the proteins responsible for hemophilia, knowledge of this structure may lead to the development of new pharmaceuticals for the treatment of this devastating disease as well as other thrombotic disorders such as stroke.

Advanced Scientific Computing Research

High performance anisotropic diffusion equation solver: Members of this project have developed a unique algorithm that, when used in conjunction with advanced medical images, can predict communication pathways in the brain. In particular, the algorithm uses solutions of the anisotropic diffusion equation to help predict converging or branching fiber tracts. Prior methods for predicting pathways stall when they reach branch points (or at the very best do not proceed down all the branches). The new algorithm easily predicts and proceeds down all branches, and could prove crucial in helping to non-invasively diagnose the onset of various brain disorders. The anisotropic diffusion equation solver requires modules from a specialized toolkit, a set of high performance computational routines developed at various DOE national laboratories.

High Energy Physics

Discovering the Higgs Bosons: The most important goal for the Fermilab Tevatron Run II and the CERN Large Hadron Collider (LHC) is the investigation of the mechanism by which elementary particles acquire mass—the discovery of the favored Higgs bosons or another mechanism. A research group at the University of Oklahoma has investigated the prospects for the discovery of a neutral Higgs boson ($\phi 0$) produced with one bottom quark $bg \to b\phi 0$ followed by Higgs decays into muon pairs within the framework of the minimal supersymmetric standard model. Promising results are found for the CP-odd (A0) and the heavier CP-even (H0) Higgs bosons. This discovery channel with one bottom quark greatly improves the LHC discovery potential beyond the inclusive channel $pp \to \phi 0 \to \mu+\mu- +X$. The muon discovery channel will provide a good opportunity for a precise reconstruction of the Higgs boson masses.

Nuclear Physics

Designing and building a polarized frozen spin target at Thomas Jefferson National Laboratory (JLab): Ordinary matter is made of protons and neutrons called nucleons, and their exact structure is still unknown. Polarized beams and targets are essential tools in the study of the nucleon. Nucleons are like small magnets and can be collectively oriented by strong magnetic fields (~5T) at low temperatures (<1K). A state of the art polarized frozen spin target has been designed and being built at JLab. It will be used to look for so called "missing resonances" (nucleon states which are predicted but have not been seen so far). This target will assist in conducting cutting edge research in nuclear physics (C. Djalali, University of South Carolina).

Renewable Energy and Efficiency

Use of Biomass: Researchers at Jackson State University are improving the amount of ethanol that can be produced from Southern pines. Acid hydrolysis is being developed for conversion of biomass into a liquid process stream (hydrolyzate) that can be either directly fermented into ethanol or further processed by enzymatic conversion into a then more fermentable stream used to make ethanol. Southern pine acid hydrolyzate containing sugars and inhibitors, such as furans and phenolics, was treated with a weak anion resin and laccase immobilized on kaolinite. Fermentation of the sugars in the treated hydrolyzate resulted in significantly higher ethanol production levels than those achieved with the untreated hydrolyzate.

Defense Programs

Robust Radiography Devices: Development of robust x-ray radiographic devices is an important need for many DOE national security applications, which require an improved understanding of electrical breakdown in high voltage insulators. To address this challenge, the Nevada Shocker (a 540,000 V pulse power machine) has been developed, and is now in operation, at the Pulsed Power Laboratory at the University of Nevada, Las Vegas. Also developed were a number of sensors and a novel calibration technique to absolutely quantify the sensor data, which measures the strength and motion of the radially propagating electromagnetic pulse interrogating the insulator under test. This will lead to basic understanding of electrical properties of insulators that are used in nuclear weapons program.

Fossil Energy

Distributed Generators: Research by West Virginia University's Advanced Power and Electricity Research Center (APERC) shows that distributed generators (DGs) such as fuel cells and microturbines can be used to "balance" electricity supply and demand at the distribution network level, opening the possibility for distribution networks to operate autonomously from the transmission system, in effect becoming "microgrids." For such microgrids to work, the DG must be able to track electricity demand in real time, producing more or less electricity to exactly meet the current demand or risk losing the network causing a blackout. Today's DGs are not able to continuously vary the amount of electricity they produce. To address this issue, APERC researchers have developed control design algorithms that would allow DGs to adjust their output and provide energy balancing in a distribution system (Richard Bajura, West Virginia University).

Mission Relevance:

The principal objective of the DOE EPSCoR program is to enhance the abilities of the designated states to conduct nationally competitive energy-related research and to develop science and engineering human resources to meet current and future needs in energy related areas. In addition, EPSCoR grants are supporting graduate students, undergraduates and postdoctoral associates, and encouraging them to be trained in world-class research at national laboratories.

Scientific Challenges:

The DOE EPSCoR activity will continue to support basic research spanning the broad range of science and technology programs within DOE.

Funding Summary (By EPSCoR States):

(Dollars in Thousands)

	FY 2005	FY 2006 Estimate	FY 2007 Estimate
Alabama	695	685	258
Alaska	0	0	0
Arkansas	145	135	139
Delaware	0	0	0
Hawaii	0	0	0
Idaho	476	375	375
Kansas	626	135	0
Kentucky	224	0	0
Louisiana	660	462	375
Maine	0	0	0
Mississippi	667	132	0
Montana	375	455	133
Nebraska	120	265	269
Nevada	0	90	105
New Hampshire*	-	0	0
New Mexico	135	135	0
North Dakota	406	273	0
Oklahoma	485	350	350
Puerto Rico	375	375	0
Rhode Island*	-	0	0
South Carolina	716	660	525
South Dakota	125	125	0
Tennessee	0	140	140
Vermont	705	0	0
U.S. Virgin Islands	0	0	0
West Virginia	315	225	135
Wyoming	270	140	140
Technical Support	123	60	110
Other**	0	2,063	4,946
Total	7,643	7,280	8,000

*New Hampshire and Rhode Island became eligible for funding in FY 2006.
**Uncommitted funds in FY 2006 and FY 2007 will be competed among all EPSCoR states.

Projected Evolution:

A solicitation for Implementation awards was issued in FY 2005, and 13 formal proposals were submitted and are under review. The program continues to meet the challenge of providing a balance between the Implementation awards and the Laboratory-State Partnership awards.

Research Activity:	**Neutron and X-ray Scattering Facilities**
Division:	Scientific User Facilities
Primary Contact:	Roger W. Klaffky (roger.klaffky@science.doe.gov; 301-903-1873)
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Division Director:	Pedro A. Montano

Portfolio Description:

This activity supports the operation of four synchrotron radiation light sources and three neutron scattering facilities. These are: the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL); the Advanced Photon Source (APS) at Argonne National Laboratory (ANL); the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL); the Stanford Synchrotron Radiation Laboratory (SSRL) at the Stanford Linear Accelerator Center (SLAC); the High Intensity Flux Reactor (HFIR) at Oak Ridge National Laboratory (ORNL); the Intense Pulsed Neutron Source (IPNS) at ANL; the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory (LANL), and the Spallation Neutron Source (SNS) at ORNL, which is a next-generation short-pulse spallation neutron source that will be significantly more powerful than the best spallation neutron source now in existence—ISIS at the Rutherford Laboratory in England. Under construction is the Linac Coherent Light Source (LCLS) at SLAC, which is a free-electron laser that will provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude greater in peak power and peak brightness than any existing coherent x-ray light source. R&D is underway on the NSLS-II which will be built as a replacement for NSLS-I to enable the study of material properties and functions at the nanoscale level and to provide the world's finest x-ray imaging capabilities.

Unique Aspects:

The synchrotron radiation light sources and the neutron scattering facilities are the most advanced facilities of their kind in the world. Together, they serve more than 7,000 users annually from academia, Department of Energy (DOE) national laboratories, and industry, a number that has more than tripled in the past decade and that can more than double again in the next decade as current facilities and those under construction are fully instrumented. These light sources and neutron scattering sources represent the largest collection of such facilities operated by a single organization in the world. Conception, design, construction, and operation of these facilities, which in current costs are in the hundreds of millions to in excess of a billion dollars, are among the core competencies of the BES program.

Relationship to Other Programs:

This activity has very strong interactions with all BES programmatic research that use synchrotron and neutron sources. This includes research in atomic physics, condensed matter and materials physics, chemical dynamics, catalysis, geosciences, high-pressure science, environmental sciences, engineering, biosciences, and much more. Interaction also exists with other parts of the Office of Science, notably the Office of Biological and Environmental Research, and DOE, notably the National Nuclear Security Administration, the Office of Energy Efficiency and Renewable Energy, and the Office of Environmental Management. There are frequent contacts with other federal agencies in order to better coordinate efforts in optimizing beamlines and instruments. This activity participates in a number of Office of Science and Technology Policy (OSTP) and National Science and Technology Council (NSTC) interagency activities, e.g., OSTP Interagency Working Groups on macromolecular crystallography at the synchrotron light sources and on neutron sources and instrumentation. This activity is establishing more frequent contacts with international user facilities such as ESRF, SPring-8, ILL, ISIS, and others. The objective is to share experiences and to make optimal use of present facilities.

Significant Accomplishments:

The synchrotron radiation light sources. During the past two decades, BES has been the nation's major supporter of synchrotron x-ray light sources. BES support pioneered new storage ring lattices for improved beam stability and brightness; developed wiggler and undulator insertion devices that provide 10-12 orders of magnitude greater brightness than the best conventional x-ray sources; and discovered or developed such powerful experimental techniques as magnetic x-ray scattering, microbeam diffraction, x-ray microscopy, photoelectron spectroscopy and holography, inelastic x-ray scattering using nuclear resonances, extended x-ray absorption fine structure (EXAFS), and near-edge absorption fine structure (NEXAFS). The BES light sources are used by over 6,500 researchers annually from academia, government laboratories, and industry for state-of-the art studies in materials science, physical and chemical science, geoscience, environmental science, bioscience, medical science, and pharmaceutical science. Recent research at the light source facilities, supported by BES, by other agencies, by industry, and by private sponsors includes: high-resolution imaging of precision-fabricated thin films of copper, pointing the way toward much denser magnetic data storage for computers; imaging of contaminants in a polycrystalline silicon solar cell and their removal by heat treatment—a step toward more efficient, less costly solar cells; development of a high-pressure "diamond anvil cell" enabling the creation of entirely new classes of materials such as biomaterials, semiconductor phases, and dense polymers; the solution of the structure of HIV (the AIDS virus) laying the groundwork for developing a vaccine; and the determination of the structure of a key (immunoglobulin-E) antibody receptor on immune system cells, opening the way to prevention of allergic reactions.

The neutron scattering sources**.** Since the late 1940s, BES and its predecessors have been the major supporter of neutron science in the United States--from the earliest work of Clifford Shull and E. O. Wollan at ORNL's Graphite Reactor in the 1940s to the Nobel Prize in Physics shared by Clifford Shull and Bertram Brockhouse in 1994 for their work on neutron scattering. Based on its experience in nuclear reactors and particle accelerators over the years, DOE developed research reactors and spallation sources as high-flux neutron sources for spectroscopy, scattering, and imaging and helped pioneer virtually all the instruments and techniques used at these facilities. Researchers at ANL, BNL, and ORNL led these pioneering advances. Most of the important techniques used today have been developed at ANL, BNL, and ORNL. Neutron scattering provides important information on the positions, motions, and magnetic properties of solids. Neutrons possess unique properties such as sensitivity to light elements, which has made the technique invaluable to polymer, biological, and pharmaceutical sciences. Neutrons also have magnetic moments and are thus uniquely sensitive probes of magnetic interactions; neutron scattering studies have led to higher strength magnets for more efficient electric generators and motors and to better magnetic materials for magnetic recording tapes and computer hard drives. Finally, the high penetrating power of neutrons allows nondestructive property measurements deep within a specimen and has been used to study automotive gears and brake discs, and defects in airplane wings, engines, and turbine blades.

Mission Relevance:

These facilities were born from the most fundamental of needs, i.e., the need to characterize materials at the atomic and molecular level. In order to understand, predict, and ultimately control materials properties, it is necessary to determine the atomic constituents of materials, the positions of the atoms in materials, and how the materials behave under the influence of external perturbations such as temperature, pressure, chemical attack, and excitation by photons, electrons, and other particles. A large number of experimental and theoretical tools are used to achieve these ends. In the last two decades, the experimental demands have motivated the development of centralized facilities, like the ones in existence for synchrotron radiation and neutron scattering. Such highly sophisticated and expensive tools are by nature centralized and staffed with specialists that provide to the user community expertise in order to optimize the scientific use of the facility. The development, construction and operation of these facilities are one of the most important missions and core competencies of BES. The scientific accomplishments of these facilities, as determined by triennial peer review, are reflected in the large number of publications appearing annually in the most important scientific journals, in the thousands.

Scientific Challenges:

The synchrotron radiation light sources. First, completion of SPEAR3 at SSRL requires upgrading the beamlines to make full use of the new more powerful radiation source. Second, the facilities must be operated optimally, which means optimizing instrument-hours of operation, not just accelerator hours of operation, and making the instruments widely available to the general user community. Third, the promise of a coherent, short-wavelength x-ray source from the LCLS will require completely new instrument and experiment concepts.

The neutron scattering sources. First, the upgrades and new instrumentation at HFIR must be completed in a timely way to facilitate a robust user program. Second, the SNS must successfully perform its commissioning and early operational phases.

Funding Summary:

Dollars in Thousands

	FY 2005	FY 2006	FY 2007 Request
Advanced Light Source	44,800	42,783	49,802
Advanced Photon Source	100,500	95,890	108,604
National Synchrotron Light Source	36,750	36,196	40,763
Stanford Synchrotron Radiation Laboratory	32,388	25,475	35,836
High Flux Isotope Reactor	46,900	43,330	51,598
Intense Pulsed Neutron Source	16,800	15,500	18,531
Manuel Lujan, Jr. Neutron Scattering Center	9,588	10,000	10,582
Spallation Neutron Source	37,600	101,001	171,409
REDC	4,500	---	---
Neutron and X-ray Scattering Facilities, Total	329,826	370,175	487,125

Projected Evolution:

X-ray and neutron scattering will continue to play a central role in the growth of BES programmatic science. The facilities will need continuous growth in terms of beamline upgrades, new neutron scattering instruments, and increase in availability of user time. The set of instruments associated with these facilities provides unique scientific and technical capabilities, rarely available in other parts of the world. These facilities need to be kept in an optimal operational mode in order to maintain and increase the tremendous scientific achievements they have facilitated.

The instrumentation and scientific needs required by the future operation of the SNS at ORNL will be identified and addressed. The SNS will be for years to come the most important neutron spallation source in the world. It is important to be prepared for full use and judicious increases in the capabilities of SNS as recommended by all advisory committees to DOE.

Finally, the LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 orders of magnitude greater than current synchrotrons; the light is coherent or “laser like” enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length) enabling studies of fast chemical and physical processes. These characteristics open new realms of scientific applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.

Research Activity:	**Nanoscience Centers**
Division:	Scientific User Facilities
Primary Contact(s):	Kristin A. Bennett (Kristin.Bennett@science.doe.gov; 301-903-4269) Altaf (Tof) Carim (carim@science.doe.gov; 301-903-4895)
Division Director:	Pedro A. Montano

Portfolio Description:

This activity supports the establishment and operation of five Nanoscale Science Research Centers (NSRCs) at Department of Energy (DOE) national laboratories. These are: the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL); the Molecular Foundry at Lawrence Berkeley National Laboratory (LBNL); the Center for Integrated Nanotechnologies (CINT) at Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL); the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (ANL); and the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL). The first four of these will be in full operation in FY 2007 and the fifth in FY 2008. All encompass state-of-the-art equipment and expert staff to support the synthesis, processing, fabrication, and analysis of materials at the nanoscale. The NSRCs are major user facilities serving researchers from academia, national laboratories, and industry and are anticipated to collectively serve over 800 users annually once all are in full operation.

Unique Aspects:

Nanotechnology is the understanding and control of matter at dimensions of roughly 1 to 100 nanometers, where unique phenomena enable novel applications. With a nanometer corresponding to one billionth of a meter, nanoscale phenomena occur at the level of small numbers of atoms, molecules, and supramolecular structures. The NSRCs will make sophisticated research tools for nanoscience and nanotechnology available to the broad scientific community, and will facilitate access to other collocated major facilities including synchrotron radiation light sources, neutron scattering centers, and electron beam microcharacterization facilities. The NSRCs are the DOE signature activity in nanoscale research and constitute the nation's largest scientific infrastructure investment under the National Nanotechnology Initiative (NNI).

NSRCs provide unique scientific and engineering capabilities not available in any of the parallel programs sponsored by other entities. For example, other federal agencies sponsor research in nanoscience at universities, but such program are generally limited in scope and size, centered on specific research issues or topical areas, and primarily involve researchers of the host institution and a limited number of partners. The NSRCs are larger-scale facilities with a broad remit and range of capabilities and are broadly accessible without usage fees for non-proprietary work, with instrument time and staff support allocated on the basis of peer-review of proposals. The purposes of the NSRCs are as follows:

- Advance the fundamental understanding and control of materials at the nanoscale regime
- Provide an environment to support research of a scope, complexity, and disciplinary breadth not possible under traditional individual investigator or small group efforts
- Provide the foundation for the development of nanotechnologies important to DOE
- Provide state-of-the-art equipment to in-house laboratory, university, and industry researchers and optimize the use of national user facilities for materials characterization employing electrons, photons, and neutrons
- Provide a formal mechanism for both short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers
- Provide training for graduate students and postdoctoral associates in interdisciplinary nanoscale science, engineering, and technology research

Relationship to Other Programs:

The fundamental science being carried out at the NSRCs is closely related to BES programmatic research on the nanometer scale at both universities and national laboratories. Researchers supported by BES, by other parts of the Office of Science, by other parts of DOE, and by other federal agencies participate in the overall NSRC user community. A major benefit is the opportunity for users to collaborate with the NSRC scientists. In addition, the NSRCs are collocated with, and serve as access points to, existing major BES user facilities for x-ray, neutron, and electron scattering. The DOE nanoscience activities as a whole are coordinated with other agencies through the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology

Council (NSTC); this Subcommittee is responsible for the federal NNI program and is currently co-chaired by representatives from BES and the Office of Science and Technology Policy.

Significant Accomplishments:

Physical construction of new buildings is complete or nearly so for four of the five NSRCs, constituting major progress in the challenging process of establishing these facilities. All five have had robust pre-operations "jump-start" user programs in which existing capabilities of the host laboratories were made available to outside users as a prelude to operations of the NSRCs themselves. Over 400 user proposals were accommodated during this period, leading to substantial advances in a number of areas; a few examples include the development and application of methods for the controlled synthesis of hollow or filled nanospheres; new insights on charge transport within two-dimensional and quasi-one-dimensional nanocrystal arrays; and the development of modular microlaboratories that facilitate sophisticated, reproducible measurement of the behavior and properties of nanomaterials.

Mission Relevance:

A part of the mission of the Office of Science is to "deliver the premier tools of science to our Nation's research enterprise." The NSRCs join the suite of major DOE user facilities that fulfill this objective. A seminal DOE-BES workshop and subsequent report on *Basic Research Needs to Assure a Secure Energy Future* cited nanoscience as a critical cross-cutting theme, and this has been reiterated in follow-up reports on *Basic Research Needs for the Hydrogen Economy* and *Basic Research Needs for Solar Energy Utilization*. In addition, BES and the NSTC cosponsored a major workshop and report on *Nanoscience Research for Energy Needs* that identified key research targets and foundational themes for energy-related nanoscience. As stated in the Executive Summary of that report, "At the root of the opportunities provided by nanoscience to enhance our energy security is the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, chemical reactions, etc.) take place on the nanoscale."

Scientific Challenges:

Strategic investments in scientific areas of opportunity are required to help our nation develop a balanced research and development infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the new century. Nanotechnology R&D is a top federal priority with broad potential implications for the nation's competitiveness. DOE's response has been the development of the NSRCs, whose goals include: (1) to attain a fundamental scientific understanding of nanoscale phenomena, particularly collective phenomena; (2) to achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions; (3) to take full advantage of other existing major user facilities, and (4) to develop experimental characterization techniques and theory/modeling/simulation tools necessary to drive the nanoscale revolution.

There are a large number of scientific challenges, all of which involve the collocation of disparate disciplines in order to fabricate and assemble nanosized components. One of the most challenging scientific problems is interfacing hard and soft matter, i.e., the world of electronic and structural materials with the world of biomaterials. These centers will employ advanced experimental and theoretical tools to tailor and control the functionality (e.g., detection ability and sensitivity), compatibility, performance, and integration of materials at such interfaces.

Funding Summary:

	Dollars in Thousands		
	FY 2005	FY 2006	FY 2007 Request
Construction:			
Other Project Costs	600	993	500
Project Engineering and Design	1,996	0	0
Center for Nanoscale Materials, ANL	12,000	14,000	0
Center for Nanophase Materials Sciences, ORNL	17,669	0	0
The Molecular Foundry, LBNL	31,828	9,510	257
Center for Integrated Nanotechnologies, SNL/LANL	30,650	4,580	247
Center for Functional Nanomaterials, BNL	18,317	36,187	18,864
Operation:			
Center for Nanoscale Materials, ANL	0	3,500	19,190
Center for Nanophase Materials Sciences, ORNL	0	17,800	19,190
The Molecular Foundry, LBNL	0	8,100	19,190
Center for Integrated Nanotechnologies, SNL/LANL	0	11,900	19,190
Center for Functional Nanomaterials, BNL	0	0	0
TOTAL	113,060	106,570	96,628

Projected Program Evolution:

The NSRCs are transitioning to standard user operations within the new facilities and with their initial suite of specialized technical equipment. The completion of this process will bring major new resources on-line for users, including nanoprobe beamlines at synchrotron radiation sources, extensive cleanroom facilities, nanoscale electron beam writers, and extensive nanomaterials synthesis and assembly capabilities. User programs will expand and adapt to respond to the needs of the community. The NSRCs are expected to perform as world-leading institutions, excelling both in scientific impact and productivity and in working with users.

Research Activity: Electron-beam Microcharacterization

Division: Scientific User Facilities
Primary Contact(s): Altaf (Tof) Carim (carim@science.doe.gov; 301-903-4895)
Division Director: Pedro A. Montano

Portfolio Description:

This activity supports three electron-beam microcharacterization user centers: the Electron Microscopy Center for Materials Research (EMC) at Argonne National Laboratory (ANL); the National Center for Electron Microscopy (NCEM) at Lawrence Berkeley National Laboratory (LBNL); and the Shared Research Equipment Program (SHaRE) at Oak Ridge National Laboratory (ORNL). These centers contain a variety of highly specialized instruments to provide information on the structure, chemical composition, and properties of materials from the atomic level on up, using direct imaging, diffraction, spectroscopy, and other techniques based primarily on electron scattering. They accommodate over 500 users annually and also participate in leading-edge instrument development. These three facilities, along with two other BES-funded efforts, collaborate on the Transmission Electron Aberration-corrected Microscope major item of equipment project to develop a next-generation platform for electron microscopy and an initial instrument optimized for high resolution and atomic tomography.

Unique Aspects:

Electron probes are ideal for investigating local structure and chemistry in materials because of their strong interactions with atomic nuclei and bound electrons, allowing signal collection from small numbers of atoms–or, in certain cases, just one. Furthermore, the use of these charged particles allows electromagnetic control and lensing of electron beams resulting in spatial resolution that can approach single atomic separations or better (i.e., approaching or exceeding 0.1 nm). The BES electron-beam characterization user facilities provide unparalleled access to specialized equipment and expert staff and develop next-generation instrumentation and characterization techniques. They make these capabilities available to the scientific community on the basis of submitted proposals and at no cost to non-proprietary users, and are the only facilities of this type focused on electron-beam characterization that are available in the nation.

Relationship to Others:

These activities couple with many others in BES programs and enable a broad range of research across numerous fields, including physics, chemistry, and materials science, within national laboratory programs as well as for academic and other scientists. The most direct relationship is with the Structure and Composition of Materials program, of which this was a part prior to FY 2007. There are also strong interactions with other BES user facilities, particularly with the collocated Nanoscale Science Research Centers. The electron-beam centers support use by researchers funded by BES, by other parts of the Office of Science, by other parts of the Department of Energy, and by numerous other federal agencies.

Significant Accomplishments:

Major historical accomplishments for the electron-beam characterization centers have included the development and operation of the Atomic Resolution Microscope (in the early 1980s) and One-Angstrom Microscope (in the late 1990s) at NCEM, which have been world-leading instruments in demonstrated lateral spatial resolution. Extensive in-situ work on radiation damage in materials has been done in unique facilities at EMC, which has operated several TEMs attached directly to ion accelerators. The SHaRE program has emphasized chemical identification and spectroscopy, with notable achievements in pinpointing the elemental segregation phenomena leading to brittleness or toughening behavior at ceramic interfaces and in developing and using novel methods and tools such as atom location by channeling-enhanced microanalysis (ALCHEMI) and the local electrode atom probe (LEAP). Recent scientific advances have included measurement of picometer-level atomic displacements, structural determination of nanoscale particles and novel defect structures such as "chevron" features at grain boundaries, and application of microcalorimetry to vastly improve energy resolution in localized analysis within multiphase superalloys and interplanetary dust particles.

Mission Relevance:

Atomic arrangements, local bonding, defects, interfaces and boundaries, chemical segregation and gradients, phase separation, and surface phenomena are all aspects of the nanoscale and atomic structure of materials, which ultimately control the mechanical, thermal, electrical, optical, magnetic, and many other properties and behaviors.

Understanding and control of materials at this level is critical to developing materials for and understanding principles of photovoltaic energy conversion; hydrogen production, storage, and utilization; catalysis; corrosion; response of materials in high-temperature, radioactive, or other extreme environments; and many other situations that have direct bearing on energy, environmental, and security issues.

Scientific Challenges:

One of the current major challenges in electron beam techniques is to take the greatest possible advantage of recently-demonstrated (and still developing) capabilities for correcting the aberrations of electron microscope lenses. The opportunities includes improvement of spatial resolution, but also offer the promise of much more extensive in-situ and other capabilities as a result of increased flexibility and space in the sample stage and surrounding area. The TEAM project that the three electron-beam centers participate in is a major effort to address these prospects. Also, with extensive work already underway in nanoscience and the transition to operations of the DOE collocated Nanoscale Science Research Centers, the electron-beam facilities provide unique opportunities to interrogate local structure and chemistry at individual nanoscale features, and will be challenged to address a large variety and volume of scientific issues across the broad spectrum of this field.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
7,614	7,945	7,945

Projected Program Evolution:

The electron-beam characterization facilities were previously supported within BES research programs and in FY 2007 come under the category of scientific user facilities, with corresponding formal responsibilities for both scientific excellence and user productivity and satisfaction. Further development will be driven by the scientific needs of users and will involve suitable renewal of instrumentation and a continued increase in interactions with other BES user facilities.

Research Activity: Transmission Electron Aberration-corrected Microscope (TEAM)

Division:	Scientific User Facilities
Primary Contact(s):	Altaf (Tof) Carim (carim@science.doe.gov; 301-903-4895)
Division Director:	Pedro A. Montano

Portfolio Description:

The TEAM project is a Major Item of Equipment project to construct and operate a new aberration-corrected electron microscope and make this capability widely available to the materials and nanoscience communities. The projected improvement in spatial resolution, contrast, sensitivity, and the flexibility of design of electron optical instruments will provide unprecedented opportunities to observe directly the atomic-scale order, electronic structure, and dynamics of individual nanoscale structures. The TEAM instrument will be optimized for high-resolution imaging and atomic tomography. The components and approaches developed will further provide a platform for future aberration-corrected instruments optimized for different purposes such as wide-gap in-situ experimentation, ultimate spectroscopy, ultrafast high-resolution imaging, synthesis, field-free high resolution magnetic imaging, diffraction and spectroscopy, and other extremes of temporal, spectral, spatial or environmental conditions.

Unique Aspects:

Transmission electron microscopy represents one of the few methods for obtaining local information with a spatial resolution of 0.1 nm or better from individual nanometer-scale structures. Aberrations of the electromagnetic lenses are the primary limitation on electron microscope resolution and constrain other aspects of the instrument including available space for in-situ manipulation in the sample chamber. The TEAM instrument is expected to attain direct spatial resolution of 0.05 nm, which is better than has been demonstrated for any present instrument. The project aims to redesign the transmission electron microscope around aberration-corrected optics, to develop a common platform for a powerful new nanocharacterization instrument, and to make this instrument widely available to the materials and nanoscience community via existing BES user facilities.

Relationship to Other Programs:

The project involves a collaboration of the three BES user facilities for Electron Beam Microcharacterization (at Lawrence Berkeley National Laboratory (LBNL), Argonne National Laboratory, and Oak Ridge National Laboratory) and two other BES-supported microscopy groups (at Brookhaven National Laboratory and at the University of Illinois at Urbana-Champaign). The lead organization and institution of the principal investigator is LBNL, and the completed instrument will be installed and operated within the National Center for Electron Microscopy (NCEM) at LBNL.

Mission Relevance:

The need and scientific case for TEAM have been vetted by the Basic Energy Sciences Advisory Committee (BESAC) and subgroups of BESAC on several occasions, including a review in 2000, an update in 2002, and a 2003 assessment of facilities roadmapping. The project was subsequently included as a near-term priority in the Department of Energy (DOE) Office of Science report, *Facilities for the Future of Science: A Twenty-Year Outlook*, in November 2003. Upon completion this instrument will become part of an existing user facility, the NCEM at LBNL, and will be available to users. The development of this equipment thus is relevant to a broad range of BES research elements, and has most direct impact on and interaction with the activities in Electron-beam Microcharacterization, Structure and Composition of Materials, and Nanoscience Centers.

Scientific Challenges:

A wide variety of major scientific challenges that could be uniquely addressed by electron scattering methods were outlined by keynote speakers at a series of workshops convened to discuss and determine the parameters for the TEAM project. These included:

- Synthesis and assembly of nanomaterials, and an understanding of their properties, especially through local electronic structure determination
- Numerous nanoscale materials issues that currently define the end of the roadmap in silicon-based semiconductor technology
- Atomic-scale origins of magnetism at the nanoscale
- Role of individual dopants and point defects in solid-state lighting materials, such as GaN

- Direct comparison of theory and experiment at the nanoscale, through the determination of the three-dimensional atomic-scale structure of nanostructures
- Atomic-scale mechanisms of controlled chemical processes/catalysis
- Size effects on thermodynamic properties of nanostructures
- Role of oxygen in high-temperature superconductivity
- Atomic-scale mechanisms of oxidation and corrosion
- Direct high-resolution imaging of biological materials and of the interface between hard and soft materials

These challenges provide scientific drivers for the TEAM project. While fulfilling all of these is not expected, the desired outcome for TEAM is to address a number of these grand challenges in full or in part.

Funding Summary:

	Dollars in Thousands		
	FY 2005	FY 2006	FY 2007 Request
TEAM Major Item of Equipment	5,586	6,206	5,508

Projected Evolution:

As for any instrumentation or construction effort of this magnitude, the TEAM project is managed in accordance with DOE Order 413.3, Project Management for the Acquisition of Capital Assets, which sets out procedures and major milestones in the form of critical decisions (CDs). Mission Need (CD-0) for the TEAM project was approved in June 2004; approval of the formal Acquisition Strategy and of CD-1 (Alternative Selection and Cost Range) followed in October 2005. The microscope will be designed and built on a phased schedule. An initial instrument incorporating spherical aberration correction, as well as a novel electron gun and sample chamber arrangement, is expected to be available to users in 2008. The final instrument will incorporate a more advanced corrector under development (addressing both spherical and chromatic aberration) and is to be commissioned and made available to users in 2009.

Research Activity: Accelerator and Detector Research

Division: Scientific User Facilities
Primary Contact: Roger W. Klaffky (roger.klaffky@science.doe.gov; 301-903-1873)
Division Director: Pedro A. Montano

Portfolio Description:

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Research seeks to achieve a fundamental understanding beyond the traditional accelerator science and technology to develop new concepts to be used in the design of new accelerator facilities for synchrotron radiation and spallation neutron sources. Research includes studies of the creation and transport of ultra-high brightness electron beams to drive Self Amplified Spontaneous Emission (SASE) Free Electron Lasers (FELs) such as the Linac Coherent Light Source (LCLS). Collective electron effects as micro-bunch instabilities from coherent synchrotron and edge radiation are key areas of interest as they can degrade the beam brightness. Beam bunching techniques such as magnetic compression or velocity bunching are also vital to the operation of the LCLS and other FELs. Research is supported to develop fast THz measurement instruments which will determine the longitudinal and transverse structure of femtosecond electron bunches leading to an increase in tuning speed of the various bunch compressive stages at the LCLS. The Accelerator Test Facility (ATF) at Brookhaven National Laboratory (BNL) is partially supported so that studies in these areas can be carried out. In the area of neutron science, there is research to develop improved high intensity, low emittance proton sources for the Spallation Neutron Source (SNS) and other accelerator-driven neutron sources such as the Los Alamos Neutron Science Center (LANSCE). More efficient proton sources can increase the reliability and lifetime due to lower RF power requirements. To exploit fully the fluxes delivered by synchrotron radiation facilities and the SNS, new detectors capable of acquiring data several orders of magnitude faster are required. Improved detectors are especially important in the study of multi-length scale systems such as protein-membrane interactions as well as nucleation and crystallization in nanophase materials. They will also enable real-time kinetic studies and studies of weak scattering samples.

Unique Aspects:

The accelerator and detector research is carried out to improve the output and capabilities of synchrotron radiation light source and the neutron scattering experiments at facilities that are the most advanced of their kind in the world. Together, they serve more than 7,000 users annually from academia, Department of Energy (DOE) national laboratories, and industry, a number that has more than tripled in the past decade and that can more than double again in the next decade as current facilities and those under construction are fully instrumented. These light sources and neutron scattering sources represent the largest collection of such facilities operated by a single organization in the world. Conception, design, construction, and operation of these facilities, which in current costs are in the hundreds of millions to in excess of a billion dollars, are among the core competencies of the BES program.

Relationship to Other Programs:

This activity strongly interacts with BES programmatic research that uses synchrotron and neutron sources. This includes research in atomic physics, condensed matter and materials physics, chemical dynamics, catalysis, geosciences, high-pressure science, environmental sciences, engineering, biosciences, and much more. It also interacts with other DOE offices, especially in the funding of capabilities whose cost and complexity require shared support. The BNL ATF is jointly funded by the High Energy Physics (HEP) Program and BES. There is also collaboration with the National Science Foundation (NSF) on Energy Recovery Linac (ERL) research. There is a coordinated effort between DOE and NSF to facilitate the development of x-ray detectors. There are ongoing industrial interactions through DOE Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) Program awards for the development of x-ray detectors.

Significant Accomplishments:

Bunch compression and coherent radiation studies at the ATF using a University of California at Los Angeles (UCLA) chicane have led to the first observation of multi-THz coherent edge radiation. Measurements of phase space distortions from acceleration fields have been carried out and will serve as a basis for FEL bunch length diagnostics. A holographic THz Fourier transform spectrometer test bed at Thomas Jefferson National Accelerator Facility was completed, the first required step for developing single shot device to completely characterize bunch shapes. Both of these diagnostic advances are targeted towards the LCLS. Other research relevant to the SNS includes the development of an advanced ^{3}He neutron detector prototype that has shown that the ionization mode works in two-dimensions for thermal neutron detection and is capable of measuring pulse height distributions with the best ever energy resolution in this mode. Gigabyte per second data rates will be achievable from this device. There were also advances in developing a higher output, high brightness H^- source for the SNS that circumvents RF antennae issues. Highly promising results have been obtained by extracting H^- ions directly from a microwave-driven plasma behind an electrostatic screen filter. The H^- ion current extracted was three times higher that of the present SNS source at comparable power.

Mission Relevance:

This research supports the most fundamental of research needs, i.e., the need to characterize materials at the atomic and molecular level. In order to understand, predict, and ultimately control materials properties, it is necessary to determine the atomic constituents of materials, the positions of the atoms in materials, and how the materials behave under the influence of external perturbations such as temperature, pressure, chemical attack, and excitation by photons, electrons, and other particles

Scientific Challenges:

- The development of new accelerator concepts is crucial to the design and upgrade of synchrotron light sources and neutron scattering facilities.
- In the design and commissioning of new FELs such as the LCLS, experimental studies must be conducted on the creation and transport of ultra-high brightness electron beams to drive SASE.
- Start-to-end simulations of the SASE electron source, transport, and SASE FEL give details of the physics mechanisms and provide benchmark models for the x-ray FEL.
- New detectors capable of using the high data rates associated with high brightness sources will increase beamline efficiencies and user throughput.
- Detectors must also be developed that are capable of acquisition of all required x-ray data from a single femtosecond LCLC pulse.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
4,000	2,119	3,000

Projected Evolution:

X-ray and neutron scattering will continue to play a central role in the growth of BES programmatic science. The facilities will need continuous growth in terms of accelerator upgrades, and x-ray and neutron detectors to fully exploit the high fluxes of x-rays and neutrons. The set of instruments associated with these facilities provides unique scientific and technical capabilities, rarely available in other parts of the world. These facilities need to be kept in an optimal operational mode in order to maintain and increase the tremendous scientific achievements they have facilitated.

The SNS will be for years to come the most important neutron spallation source in the world. It is important to be prepared for full use and judicious increases in the capabilities of the SNS as recommended by all advisory committees to DOE. Accelerator and detector research will enable these upgrades.

The instrumentation and scientific needs required by the future operation of the LCLS at the Stanford Linear Accelerator Center need to be identified and addressed. Finally, the LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 orders of magnitude greater than current synchrotrons; the light is coherent or “laser like” enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length) enabling studies of fast chemical and physical processes. These characteristics open new realms of scientific applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.