Office of Science

Basic Energy Sciences

Core Research Activities

June 2008

Office of Basic Energy Sciences

Harriet Kung, Assoicate Director
Vacant, Administrative Specialist

BES Budget and Planning
- Robert Astheimer, Technical Advisor
- Margie Davis, Budget Analyst

BES Operations
- Richard Burrow, DOE Technical Office Coordination
- Don Freeburn, DOE and Stakeholder Interactions
- Ken Rivera, Laboratory Infrastructure/ES&H
- Karen Talamini, Program Analyst/BESAC

Materials Sciences and Engineering Division
Aravinda Kini, Acting Director
Christie Ashton, Program Analyst
Charnice Waters, Secretary

- **Materials Discovery, Design, and Synthesis** — Aravinda Kini; K. Gorey, Prog. Asst.
  - Materials Chemistry: Richard Kelley; ■ James McBreen, BNL
  - Biomolecular Materials: Aravinda Kini; Vacant
  - Synthesis and Processing: Tim Fitzsimmons; Bonnie Gersten; ◆ Daniel Friedman, NREL
  - Tech. Coordination Program Management: John Vetrano
- **Condensed Matter and Materials Physics** — Jim Horwitz; M. Agnant, Prog. Asst.
  - Exp. Cond. Mat. Phys.: Andrew Schwartz; ● D. Finnemore, Ames; ◆ Daniel Friedman, NREL
  - Theo. Cond. Mat. Phys.: △ Arun Bansil, NEU; ■ James Davenport, BNL; ● Kim Ferris, PNNL
  - Physical Behavior of Materials: Refik Kortan
  - Mechanical Behavior and Radiation Effects: John Vetrano
- **Scattering & Instrumentation Sciences** — Helen Kerch; C. Howard, Prog. Asst.
  - X-ray Scattering: Lane Wilson
  - Neutron Scattering: Lane Wilson; Vacant
  - Electron and Scanning Probe Microscopies: Jane Zhu
  - Ultrafast Science and Instrumentation: Jim Glownia
  - Exp. Program to Stimulate Competitive Research: Tim Fitzsimmons; Vacant; ● Helen Farrell, INL

Scientific User Facilities Division
Pedro Montano, Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

- **Operations**
  - X-ray and Neutron Scattering Facilities: Roger Klaffky
  - Nanoscience Centers & E-beam Centers: Altaf (Tof) Carim
  - Accelerator and Detector R&D: Vacant
  - Facility Coordination, Metrics, Assessment: Vacant
- **Construction**
  - Linac Coherent Light Source: Tom Brown
  - NSLS II: Tom Brown
  - Spallation Neutron Source Upgrades: Tom Brown
  - TEAM: Tom Kiess
  - Instrument MIEs (SING, LUSI, etc.): Tom Kiess
  - ALS User Support Bldg: Tom Brown

Chemical Sciences, Geosciences, and Biosciences Division
Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

- **Fundamental Interactions** — Michael Casassa; R. Felder, Prog. Asst.
  - Atomic, Molecular, and Optical Sciences: Jeffrey Krause
  - Gas-Phase Chem. Phys.: Vacant; ◆ Larry Rahn, SNL; ◆ Wade Sisk, BNL
  - Condensed-phase and Interfacial Mol. Sci.: Gregory Fiechtner
  - Computational and Theoretical Chemistry: Vacant
- **Photo- and Bio-Chemistry** — Richard Greene; S. Watson, Prog. Asst.
  - Solar Photochemistry: Mark Spitler
  - Photosynthetic Systems: Vacant
  - Physical Biosciences: Vacant; ◆ Robert Stack, PNNL
- **Chemical Transformations** — John Miller; T. Russ, Prog. Asst.
  - Catalysis Science: Raul Miranda; Paul Maupin; ◆ Michael Chen, ANL
  - Heavy Element Chemistry: Lester Morss; ● Norman Edelstein, LBNL
  - Separations and Analysis: William Millman; ◆ Larry Rahn, SNL
  - Geosciences: Nicholas Woodward; ◆ Patrick Dobson, LBNL
  - Technology Office Coordination: Marvin Singer

Legend
- ◆ Detailee
- ■ Detailee, 1/2 time, not at HQ
- ● Detailee, 1/4 time, not at HQ
- △ IPA

June 2008

Research Activity: **Experimental Condensed Matter Physics**
Division: Materials Sciences and Engineering
Primary Contact(s): Andrew Schwartz (andrew.schwartz@science.doe.gov; 301-903-3535)
Team Leader: James Horwitz
Division Director: Aravinda Kini, Acting

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.

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. Research on the properties of materials in high magnetic fields is being conducted using the 100 T multi-shot magnet at the Los Alamos National Laboratory (LANL). Two major areas of research are being pursued 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 program and the National Science Foundation (NSF) support the National Academy of Science's Solid State Sciences Committee, which in turn serves as a coordinating mechanism nationally. The program has also supported topical activities at the National Academy of Sciences which included 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; 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. The 100 T multishot magnet at Los Alamos was designed and constructed under the ECMP program and currently holds the world record for long pulse, high magnetic fields in a reusable magnet.

Mission Relevance:

This activity provides direct research assistance to the technology program in OE on superconductivity. This activity provides direct research assistance to the technology program in EERE on photovoltaics for solar energy conversion. 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 2007	FY 2008	FY 2009
42,720	40,720	50,509

Performer	Funding Percentage*
DOE Laboratories	70%
Universities	30%

*Based on FY2007
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, terahertz, 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 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: Theoretical Condensed Matter Physics

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

Portfolio Description:
The Theoretical Condensed Matter Physics 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 four collaborative research projects: Multiscale Studies of the Formation and Stability of Surface-Based Nanostructures; Predictive Capability for Strongly Correlated Systems (an attempt to advance capabilities in many body theory); Dynamics and Cohesion of Materials Interfaces and Confined Phases Under Stress; and Multiscale Simulation of Thermo-mechanical Processes in Irradiated Fission-reactor Materials.

Relationship to Other Programs:
This activity interacts with all the other research activities within the BES Materials Sciences 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 Office of Advanced Scientific Computing Research (ASCR). 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 collaborative 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 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 materials 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 2007	FY 2008	FY 2009
23,208	25,832	36,190

Performer	Funding Percentage*
DOE Laboratories	54%
Universities	46%

*Based on FY2007

The program provides funding for >100 university grants. 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 ASCR 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: Mechanical Behavior and Radiation Effects

Division: Materials Sciences and Engineering
Primary Contact(s): John Vetrano (john.vetrano@science.doe.gov; 301-903-5976)
Team Leader: James Horwitz
Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research to understand the formation and motion of defects in materials and their effect on strength, structure, deformation, and failure. Energy-relevant materials from large-scale nuclear reactor components to nano-scale switches undergo mechanical stress and may be subjected to ionizing radiation. It is therefore important to elucidate their response to these conditions to enable the advancement of high-efficiency and safe energy generation, utilization, storage, and transportation systems. The objective of this research area is to achieve a complete understanding of the relationship between mechanical behavior and defects in materials, including defect formation, growth, migration, and propagation. Research supported in this area includes understanding deformation of ultra-fine scale materials, understanding radiation-resistant materials, and intelligent microstructural design of materials for increased strength, formability and fracture resistance. This research aims to build on this understanding in order to develop predictive models for the design of materials having superior mechanical properties and radiation resistance. A key aspect of this area will also include the development of new techniques for studying mechanical behavior and radiation resistance using the major BES scientific user facilities such as the high-brightness light sources, neutron sources, and electron microscopes in both static and dynamic conditions. Research in this topical area underpins DOE research in areas such as nuclear energy, energy efficiency, and defense programs.

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, renewable energy, 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 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 Electron and Scanning Probe Microscopies 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. The radiation aspect of this activity interacts closely with a related Computational Materials Science Network project in the Theoretical Condensed Matter Physics program. Principal investigators use BES scientific 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:

New Materials for Radiation Environments. Materials capable of resisting damage from intense radiation are essential for advanced nuclear energy systems. The primary radiation-damage mechanism in materials involves the creation and accumulation of structural defects such as atomic dislocations, vacancies, and other anomalies. Multiple defects could lead to the collapse of the ordered crystalline structure of the material, adversely affecting the integrity of material components used in nuclear energy systems. Recent studies have shown that materials can be made radiation-damage resistant by creating structures that actually accommodate radiation-induced structural disorder on the atomic scale. Complex oxides are candidate materials for these structures because they exhibit strong tendencies for natural atomic disordering. As a result, the formation of radiation-induced defects causes very little structural change, allowing the crystal structure to remain mechanically intact. The materials exhibit good radiation tolerance after high-level radiation exposure. Similarly, radiation damage can be accommodated in composite materials containing a high volume fraction of nanoscale interfaces. The interfaces are found to possess a strong affinity for defects, thereby catalytically removing them from the bulk of the material. The accumulation of large numbers of defects would otherwise lead to embrittlement and loss of mechanical integrity. The research has provided fundamental insight into tailoring the atomic structure of materials to achieve substantial improvements in radiation damage tolerance.

Nanomechanics: Elasticity and Friction in Nano-objects. The development of new materials with the size of a few nanometers has opened a new field of scientific and technological research. Nanomaterials such as oxide nanobelts and semiconductor nanowires are promising building blocks in future integrated nano-electronic and photonic circuits, nano-sensors, interconnects, and electro-mechanical nanodevices. The goal is to develop faster and better communication systems and transports, as well as smarter and smaller nanodevices for biomedical applications. To reach these objectives it is crucial to answer some fundamental questions such as what are the effects that different bonding arrangements and chemical modifications have on the elastic behavior of a nano-object. In a recent study the investigators measured the Young's modulus of ZnO nanobelts with an atomic force microscope by means of the modulated nanoindentation method developed in their lab. The elastic modulus was found to depend strongly on the width-to-thickness ratio of the nanobelt, decreasing from about 100 to 10 GPa, as the width-to-thickness ratio increases from 1.2 to 10.3. This surprising behavior was explained by a growth-direction-dependent aspect ratio and the presence of stacking faults in nanobelts growing along particular crystalline directions.

Hierarchical Structures for Enhanced Properties. A method has been devised to fabricate materials that exhibit a unique combination of desirable properties: strength, toughness, and light-weight. These materials mimic the natural oyster-shell material nacre, whose strength and toughness are far in excess of those of its constituent materials. The enhanced properties result from the "hierarchical" architecture of the materials, an architecture that is extremely difficult to fabricate because it involves the overlay of structures of multiple length scales, from micrometers to nanometers. A path for the synthesis of hierarchical materials was developed by mimicking the formation of sea ice. As saltwater freezes, impurities are expelled to separate pure water from crystalline salt. Similarly, during the freezing of water-based ceramic suspensions, ceramic particles are expelled and concentrate in the spaces between the ice crystals. The ice is then sublimated away and the space between the remaining ceramic layers is filled with an inorganic (metal) material, or, as in nacre, with an organic (polymer). The technique could be used in the fabrication of composites for a myriad of applications in which strength and lightness are imperative: structural materials, armor, airplane parts, computer hardware or orthopedic implants.

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 under extreme conditions. 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.

Scientific Challenges:

Interaction between mechanical and physical behavior: How do large magnetic or electrical fields, chemical reactions and driven phase changes (amorphization under irradiation, for example) influence the mechanical response of materials, and how does stress or strain alter their physical properties? It is being increasingly recognized that there is a strong linkage between physical and mechanical behavior. This is particularly apparent in processes such as magnetoplasticity but has also been observed in metal forming, processing and sintering. Externally applied or internally generated magnetic and electric fields have been observed to influence the deformation response in a number of materials. This opens a new avenue for controlling the mechanical properties of materials.

Cooperative phenomena: What is missed when observing or modeling individual defects or processes? Often it is found that there are synergistic and system-level effects to mechanical behavior as a number of deformation processes rely on cooperative movement of defects or microstructural components. These processes include strain hardening, grain boundary sliding, and grain growth. A more broad study of mechanical behavior at a level emphasizing cooperative phenomena would yield greater insight into how materials behave under stress.

Bridging the length and time scales; modeling; and measurement from atomic to continuum: The formation and motion of defects take place over a wide range of length and time scales. In order to fully understand response of the materials it is necessary to successfully model and measure defect motion and interactions over this range of length (from sub-nanometer to millimeter) and time scales (picoseconds to seconds) in a unified manner. This includes not only improved computational methods but also improved measurement techniques for full 3-D analysis of microstructures.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
12,626	13,620	23,112

Performer	Funding Percentage*
DOE Laboratories	77%
Universities	23%

*Based on FY2007
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, physical behavior, and behavior under extreme environments will constitute an increasingly significant part of the development of 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 extreme environment of energy systems. With the emerging importance of nanoscale structures with high surface-to-volume ratios, it is appropriate to take advantage of the new, unprecedented capabilities to fabricate and test tailored structures down to the nanoscale, taking advantage of more powerful parallel computational platforms and new experimental tools.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a materials response that can be detected in-situ over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in US energy production these are issues that need to be addressed at a fundamental level.

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.

With high-end computational capability now a reality, computational materials science will play a pre-eminent role in predicting and understanding the generation, migration and interactions of defects in materials while under stress and/or irradiation. Unified models will be developed covering all length scales that will provide significant insights into how materials react to extreme conditions at a fundamental level. Mesoscale and nanoscale modeling efforts will be extended to include nanostructured materials. With the increasing power of computers and computational codes, along with unprecedented capabilities to fabricate and test nano-scale structures under extreme conditions, the time and length scales of experiments and simulations are converging and allowing new insight into mechanical behavior and radiation effects of materials.

Research Activity: **Physical Behavior of Materials**
Division: Materials Sciences and Engineering
Primary Contact: Refik Kortan (refik.kortan@science.doe.gov; 301-903-3308)
Team Leader: James Horwitz
Division Director: Aravinda Kini, Acting

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-related 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:
This activity closely interacts with all other sister programs under BES, and also, it is linked to the Center of Excellence for Synthesis and Processing of Advanced Materials and Computational Materials Sciences Network, Solid State Lighting/Building Technologies Program, Office of Energy Efficiency and Renewable Energy, Nuclear Energy Research Initiative, Energy Materials Coordinating Committee and Hydrogen Coordinating Committee. Additionally, this program interacts with the NSTC Materials Technology Subcommittee (MatTec) Interagency Working Groups on Metals, Structural Ceramics, Nondestructive Evaluation, and Nanotechnology and the OSTP Interagency Taskforce on Hydrogen R&D.

Significant Accomplishments:
This activity has had broad and significant impact in many classes of materials and phenomena. Some of the recent accomplishments include: experimentally resolving a single individual magnetic spin on an atom, using $KNbO_3$ nanowires that combines fluorescence and force microscopies; exploitation of structural bistability in liquid crystals for low energy consuming optical switches; development of predictive tools for phase stability and structure in transition-metal oxides for fuel cells; observation of "superplastic deformation" (280% of their original length) of single wall carbon nanotubes; realization of the smallest feature size (100 nanometer Gold) 3D metallic photonic crystal materials; observation of giant magnetoresistance in Mn-based full Heusler alloys; measuring thermoelectricity of a single individual molecule; and demonstration of 50-fold improvement in thermoelectric properties in silicon nanowires.

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 the Experimental and Theoretical Condensed Matter Physics program, 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 2007	FY 2008	FY 2009
25,964	25,960	33,539

Performer	Funding Percentage*
DOE Laboratories	68%
Universities	32%

*Based on FY2007

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. This program also 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.

Research Activity: Neutron and X-ray Scattering

Division: Materials Sciences and Engineering
Primary Contact(s): Lane Wilson (Lane.Wilson@science.doe.gov; 301-903-5877)
Team Leader: Helen M. Kerch
Division Director: Aravinda Kini, Acting

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.

<u>Neutron Scattering</u> - 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.

<u>X-ray Scattering</u> - The unique properties of synchrotron radiation–high flux and brightness, tunability, polarizability, and 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.

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 inelastic x-ray scattering, extended x-ray absorption fine structure (EXAFS), x-ray microscopy, microbeam diffraction, time-resolved spectroscopy, and resonant techniques providing specific chemical, magnetic, and excitation contrast in the scattering signal.

Recent accomplishments include sensitive measurements of surface segregated atomic and electronic structure in new catalysis alloys, as well as measurements of distortions in the atomic ordering resulting from the interfacial constraints on perovskites oxide films, leading to unique magnetic and electron transport behavior. Progress in understanding the rich magnetic and electronic structure of correlated electron materials continues in terms of mapping out phase boundaries and determining the nature of the competing quantum interactions behind transitions in physical properties. Refinements with in-situ techniques (including x-ray diffraction microscopy and grazing incidence surface x-ray scattering) have become more adept at probing small samples, surfaces, and interfaces under extreme processing environments of temperature, pressure, and reactive gases.

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 and how high can the temperature be for materials to remain superconducting?

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 2007*	FY 2008*	FY 2009*
38,943	38,940	52,098

Performer	Funding Percentage
DOE Laboratories	78%
Universities	22%

*Based on FY2007
Major DOE national laboratory performers include Ames, Argonne, Brookhaven, Oak Ridge, Los Alamos, and the Stanford Linear Accelerator Center.

Also supported is the operation of HPCAT (High Pressure Collaborative Access Team).

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 careful structural measurements related to materials properties.

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 such as 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. Coupled with new instrumentation will be support for new technique development that is enabled by advances in sources and detection capability.

Research Activity: **Ultrafast Science and Instrumentation**
Division: Materials Sciences and Engineering
Primary Contact(s): James H. Glownia (James.Glownia@science.doe.gov; 301-903-2411)
Team Leader: Helen Kerch
Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research in condensed matter physics and materials physics using ultrafast electron, optical (terahertz to extreme ultraviolet), and x-ray techniques and sources. Basic research to observe, control, and understand material dynamics at the "atomistic" or "quantum" level, ultimately approaching the fundamental length (Angstroms) and time (attoseconds) scales of matter, as well as to develop and apply state-of-the-art laboratory scale advanced imaging techniques exploring dynamics at the ultrafast and ultrasmall, are supported. Projects aligned with unique capabilities at Office of Science facilities are of particular interest, as are ones that can leverage, or otherwise help advance related investment areas within BES. While conventional time-averaged probes such as time-integrated spectroscopy, DC transport, or thermodynamic measurements have provided significant insight into the microscopic properties of complex materials, many novel physical properties arise from excitations out of the ground state into energetically higher states by thermal, optical, or electrical means. Applications of ultrafast science based approaches often enable a material's degrees of freedom to be temporally separated, and this is a key aspect motivating this program that gives access to cause-effect relationships in complex materials exhibiting dynamic competition between, for example, charge, lattice, spin, and orbital degrees of freedom. Quite generally, this advances new understanding of ground state properties, coupling parameters, degrees of freedom influencing transport, the nature of phase transitions (reversible and irreversible), and non-equilibrium dynamics. Thus research in this activity helps underpin the most fundamental understanding and identification of detailed mechanisms responsible for the electronic, magnetic, optical, and physical behavior of materials. A focus of this program will be placed upon new materials science (e.g., nanoscience, condensed phase molecular processes, and condensed matter physics), enabled with ultrafast techniques and technologies in this rapidly developing field. Understanding complex material properties at a predictive discovery basis level for the control, design, synthesis, fabrication, and development of new materials possessing desired properties and functionalities is the broad goal of this program.

The activity also supports ultrafast research motivated by the largest BES construction projects in recent years - the Advanced Light Source (ALS), Advanced Photon Source (APS), and the Linac Coherent Light Source (LCLS). Basic Energy Sciences is a major supporter of both the research and the instrumentation at these and other facilities. With the advent of ultrafast x-ray beams produced by such fourth generation synchrotron radiation facilities, a number of unique capabilities will become possible including real time imaging of complex material dynamic behavior. Outside of specific ultrafast instrumentation, this program also supports activities for probing the detailed nature of materials using capabilities that are more subtle, sensitive, and precise. Basic Energy Sciences recognizes that many of the sophisticated tools for materials science research are expensive and complex, often limiting an individual investigator's ability to procure operate and maintain such instrumentation. In some such cases resources will be available for small to midsize, multiuser instruments primarily located at user facilities. Here, material science inspired midscale instruments and tools to innovate and advance creative research as well as promote education and training will be supported, with an emphasis on unique capabilities to enable discovery and understanding in emerging topics.

Unique Aspects:

Conventional diffraction techniques such as x-ray, neutron, and electron diffraction are all powerful probes of the equilibrium atomic arrangement of material systems, but they are unable to follow the evolution of transient nonequilibrium structural states. The promise of ultrafast techniques in materials dynamics is to elucidate the changes in the atomic and electronic configuration of materials along dynamical pathways while they are occurring. Ultrafast techniques provide a path towards investigating phenomena approaching the fundamental timescales of electronic and atomic motion, offering a unique snap-shot into the properties of cooperative condensed matter and material systems. Such investigations can often be used to complement time-integrated spectroscopic, neutron, and x-ray based studies. For example, capabilities such as ultrafast x-ray diffraction and absorption spectroscopy, electron diffraction, and terahertz and photoelectron spectroscopy are currently being developed. A key characteristic of dynamical techniques is that the system investigated is no longer in strict thermodynamic equilibrium (this deviation might be marginal or great). The material under study may be either in an excited state whose decay into other degrees of freedom is being probed, yielding information unavailable to conventional time-averaged frequency domain spectroscopies, or in a metastable state with fundamentally different physical properties. We envision a path towards an imaging capability at the frontier of ultrafast science, enabling measurements which begin to simultaneously approach the intrinsic length (Å) and time (10^{-18} s) scales of matter. The resultant detailed understanding of the properties of materials on an ultrafast time scale enables a robust rational basis for the design and development of new materials possessing desired properties and functionalities.

Relationship to Other Programs:

The Ultrafast Science and Instrumentation program is coordinated with BES activities under Mechanical Behavior and Radiation Effects, Physical Behavior, Synthesis and Processing, X-Ray and Neutron Scattering, Condensed Matter Physics, Atomic Molecular and Optical Sciences, Chemical Physics and the Nanoscience Centers; with other DOE offices, including the National Nuclear Security Agency; and with other federal agencies through the National Nanoscience Initiative (NNI). This activity also crosscuts several recent National Research Council (of the National Academies) studies assessing opportunities in science and technology disciplines where aspects of ultrafast science can provide impact and leadership. Some such topical activities are included in two monographs from the Decadal Survey of Physics: *Controlling the Quantum World – The Science of Atoms, Molecules and Photons* and *Condensed Matter and Materials Physics – The Science of the World Around Us* as well as in *Midsize Facilities - The Infrastructure for Materials Research.* Some research in the Ultrafast Science program is aimed at a fundamental understanding of the behavior of materials that underpin DOE technologies. Improving the understanding of the physics of materials on the nanoscale is technologically significant as these structures offer enhanced properties and could lead to dramatic improvements in energy generation, delivery, utilization, and conversion technologies.

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, especially at the nanoscale, requires ever more sophisticated experimental tools to extract useful knowledge and to develop new theories for the behavior of these materials. Hence one primary strategic investment impact from the program is the ultimate ability to control the phases and structures of materials, including those which can advance nanoscale device development. New and powerful predictive understanding of materials would be enabled to advance the discovery and rational design of systems with new and desired functionalities. As examples, such a design toolset could accelerate the synthesis and fabrication of materials and devices that include high efficiency and ultrastable photovoltaics, advanced photonic and magnetic platforms, extreme radiation hardened materials, new sensors, cradle to grave green technologies, and even the exotic possibility of materials announcing fatigue and impending failure and/or self repair. Such discovery helps sustain our nation's innovation infrastructure in support of the America Competes Act. The program is also relevant to the National Nuclear Security Administration in its activity on the behavior of matter in extreme environments, especially high strain rates, pressures, and temperatures, as well as in nonproliferation through research facilitating discovery of new sensor modalities.

Scientific Challenges:

Our ability to investigate the fundamental properties of materials, for the most part, has been outpaced by the facility with which these materials can be grown. Aside from scanning nanoprobes such as the scanning tunneling microscope and the atomic force microscope (both transformational capabilities first enabling ultrasmall scale imaging), studies of nanosystems such as wires, tubes, and dots have been carried out on ensembles exhibiting a relatively wide distribution of lengths, widths, chiralities, etc. As a result, a great deal of the detailed bulk and surface electronic structure is ultimately lost in the average values such measurements produce. A Scientific Grand Challenge in this topical area is to fully exploit the promise of new materials, especially at the nanoscale, which requires an integrated and innovative design, fabrication, measurement, modeling, and theoretical effort to achieve a predictive understanding of such complex materials. Developing the ability to better understand, predict, and use the significant differences of energy states and exotic scaling laws due to surface to volume ratio effects, together with discovering how to design novel electromagnetic response(s) with enhanced transport properties, is required to accelerate the use and integration of nanostructured materials. Research to discover materials possessing emergent properties could positively impact many applications including, superconductivity, sensors, transducers, magnetic and microelectronic devices, photovoltaics, and photonic based devices using bandgap engineered structures or metamaterials.

Coherent Control - A major theme in atomic and molecular science is: If we now understand the basics of how atoms and molecules work, can we manipulate and control them in useful ways? The control of matter on the sub-nm, sub-fs, distance- and time-scales explores the limits of fundamental atomic and molecular processes, as well as the limits of optical technology. Since atoms and molecules interact with their environment entirely by means of electromagnetic fields, the preceding question specifically asks: Is it possible to "design" a pulse of light that, when incident on an atom or molecule, can precisely control its evolution in any desired way? During the past decade, as laser technology has progressed, light pulses can now be manipulated on a cycle-by-cycle basis, and the topic of "coherent control" of atoms and molecules has drawn increasing interest. Control of coherent behavior in condensed matter systems has been difficult primarily due to the fast dephasing times of electronic or excitonic states. Advances in ultrafast lasers may soon enable the application of coherent quantum control techniques, already demonstrated in gas phase atoms and molecules, to more complex condensed matter systems. From a fundamental scientific perspective, entirely new physics emerges when the quantum states of solids are coupled and manipulated by intense optical fields. Our understanding of tightly coupled light-matter systems is, however, hampered by our lack of in-situ microscopic probes. Recent and foreseeable advances in high-brightness x-ray sources create an unprecedented opportunity to micro-probe the primary event in how optical radiation manipulates matter. When we ask a light pulse to manipulate matter it accomplishes this task by driving atomic scale distortions in a material's valence charge density. These initial microscopic distortions then propagate out to drive subsequent material evolution. To date there has been no way to directly probe these transient light induced distortions to the valence charge. New experimental capabilities are required to provide fundamental insights important for learning how coherent quantum control techniques might be used to synthesis novel materials.

Studies of Correlated and Complex Materials – One of the most important aspects of contemporary condensed matter physics involves understanding strong Coulomb interactions between the large numbers of electrons in a solid. Electronic correlations lead to the emergence of unique materials properties, such as superconductivity, magnetism, heavy Fermion behavior, Bose-Einstein condensation, the formation of excitonic gases, metal-insulator transitions, and the integer and fractional Quantum Hall effects. Such materials often exhibit competition between the charge, lattice, spin, and orbital degrees of freedom, whose cause-effect relationships are difficult to ascertain. An important characteristic of these materials is the existence of several competing states, as exemplified by their complicated phase diagrams. Such electronic complexity has consequences for applications of correlated electronic materials, because not only charge (semiconducting electronic), or charge and spin (spintronics) are of relevance, but in addition the lattice and orbital degrees of freedom are active, leading to giant responses to small perturbations. Moreover, several metallic and insulating phases compete, increasing the potential for novel behavior. The electronic correlations lead to unique materials and device properties such as high-temperature superconductivity, colossal magneto-resistance, coupled electric and magnetic functionality, and large thermopower. Potential real world applications include dissipationless wires and devices from high temperature superconductors, superior thermoelectrics, enhanced memory with states stored in magnetic and electric polarization made from multiferroic manganites, and smaller, faster, more efficient electronics. A major challenge in correlated materials is to realize this enormous potential in functionality to discover, understand, and develop new multifunctional materials and devices which perform more functions, more effectively than conventional semiconductor devices. To succeed in this challenge a more complete understanding of the underlying mechanisms and phenomena in correlated materials is required to ultimately control this complexity to achieve desired functionality. The discovery of high-TC superconductivity in particular was a watershed event, leading to dramatic experimental and theoretical advances in the field of correlated-electron systems. Yet, after one of the largest research efforts ever in physics, involving hundreds of scientists, even basic properties of the cuprate high temperature superconductors, such as the pairing mechanism, linear resistivity, and pseudogap phase, are still only poorly understood. In the past, it was expected that suitably modified theories of ordinary metals would explain the unusual properties of the cuprate's normal state, but a true understanding of this complex phenomenon remains elusive and certainly will not be incremental. Just as the historical discovery of antiferromagnetism occurred in 1949, only with the advent of neutron scattering, new and improved tools must be developed to probe "hidden" correlations in these complex materials. Ultrafast spectroscopy, consequently, is playing an ever increasing role to provide insight into cause-effect relationships associated with many-body interactions in complex materials. Quite generally, important insight into ground state properties, coupling parameters, degrees of freedom influencing quasiparticle transport, the nature of phase transitions, and nonequilibrium dynamics can be obtained as ultrafast experiments naturally probe the dynamics of systems with interacting quantum degrees of freedom. From a theoretical point of view, calculating even the ground state of correlated systems, for example the simple Hubbard model of interacting electron systems, has proven essentially intractable. It would appear that computing the full quantum dynamics of correlated and complex systems far from equilibrium would be even further out of reach. The natural impulse when faced with such a challenge is to make drastic approximations at the outset, for example to treat a problem using mean field theory, or to recognize that phonons are slow compared to electrons and to treat them semiclassically or in the adiabatic approximation. In a small molecule, where electronic excitation energies are large compared to phonon energies, the adiabatic approximation, or the assumption that the total wavefunction factors into a product of an electron piece and a phonon piece, is often appropriate. However, when the molecule becomes large, for example a long carbon nanotube or a full 3D solid, the electronic excitation energies become arbitrarily small and dense, often much smaller than a typical phonon energy. It would seem that the adiabatic approximation may fail in this regime, as in fact it does. Efforts to bridge experiment, simulation, and theory, especially leveraging information accessible at the ultrafast and ultrasmall scales, will help to fill this gap.

Studies of Systems Far From Equilibrium – Dynamic material behavior that would benefit from study with high temporal resolution, especially high-fidelity, laboratory scale, single-shot approaches, include advanced diffraction and measurement techniques to identify and quantify ultrafast strain-driven processes including phonon dynamics, phase transformations, plasticity, melting and solidification, deformation twinning, solid-state chemical reactions, radiation damage, and shock propagation processes. Such observations will allow the direct measurement of certain quantities used in models and would help serve to validate various materials simulations at atomistic scales. A broader challenge is to linking across length and time scales to achieve multi-scale understanding requiring computational and experimental coordinated approaches to define materials from atomistic to bulk scales, especially under conditions far from equilibrium. For validation, the materials community needs to search for experimental techniques and modeling approaches that link scales, where directly connecting experimental and simulation spatial and temporal scales remains a critical and pivotal need. As an example, predictions of phase transformation kinetics active during shock and dynamic deformation events will ultimately follow from prediction of the atomic motions during phase transformations. Similarly, surface reactions leading to corrosion and radiolysis effects during radiation damage require linking of spatial and temporal scales. Probing the ultrafast and ultrasmall enables a direct means to benchmark predictive models at the atomistic level, as the preferred approach is to validate such models at each length scale, from the electronic and atomic-level dynamics in single crystals, to the mesoscopic interactions between grains, and finally to the bulk polycrystalline response of engineering samples. Since predictability flows from microscopic models to higher length and time scales, experimental validation at the micro-scale is required to confidently predict material properties under rapidly varying and extreme conditions at the engineering scale, where the design and simulation of a system or device is required for engineering applications.

Funding Summary: N/A

This activity is part of the Neutron and X-Ray Scattering Research Area.

Projected Evolution:

Advances in ultrafast science will be driven by the scientific opportunities presented by improved source performance and instrumentation optimized to take advantage of that performance. The ultrafast science activity will support emerging capabilities at the DOE facilities by providing instrumentation and research support. A challenge to the program is to identify and provide support for the researchers and instruments to keep the program and facilities at the forefront of science in this technologically rapidly advancing field.

Research Activity: **Electron and Scanning Probe Microscopies**

Division: Materials Sciences and Engineering
Primary Contact(s): Jane G. Zhu (jane.zhu@science.doe.gov; 301-903-3811)
Team Lead: Helen Kerch
Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research in condensed matter physics and materials science using electron scattering and scanning probe microscopy and spectroscopy techniques. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials, especially the interplay between structural, electronic and magnetic properties at the atomic and nanometer scale and the effects of structural and compositional inhomogeneities including defects, surfaces, interfaces, and precipitates. This activity also supports the continual development and improvement of novel microscopy techniques and the next-generation instrumentation including high spatial- and temporal-resolution imaging, and high energy-resolution spectroscopy techniques to enable new discoveries in materials and nanoscience based on the ability to image the structure and functionality of materials at the nanometer or atomic scale.

Unique Aspects:

Materials properties at macroscopic scale originate from microscopic details, via a hierarchy of length scales. This activity is driven by the need for quantitative characterization and understanding of materials over atomic to micron length scales. It is a major source of research in the United States that is focused on structure and properties 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 BES' Electron Beam Microcharacterization Centers and Nanoscale Science Research Centers. The portfolio includes fundamental understanding, characterization, and analysis of materials by various electron scattering and scanning probe microscopy and spectroscopy 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 Electron and Scanning Probe Microscopies program interfaces with other programs in BES, including the activities under Condensed Matter Physics, Mechanical Behavior and Radiation Effects, Physical Behavior, Synthesis and Processing, X-Ray and Neutron Scattering, Materials Chemistry and Biomolecular Materials, Catalysis, Electron-beam Microcharacterization Centers, and Nanoscience Centers; in the Office of Science through the Computational Materials Sciences Network; in DOE through the Hydrogen Fuel Initiative (HFI) and the Energy Materials Coordinating Committee (EMaCC); and in other federal agencies through the Interagency Coordination and Communications Group for Metals (NSTC/CT/MatTec), the interagency Coordinating Committee on Structural Ceramics (NSTC/CT/MatTec), and the National Nanoscience Initiative (NNI).

.

Significant Accomplishments:

World class scientific achievements in this program represent the leading U.S. capabilities for materials characterization at atomic length scale, coupled with advances in detectability limits and precision of quantitative analytical measurement for fundamental understandings of materials. Accomplishments include:

- Imaging of electronic self-organization at atomic scale was achieved through the development of atomic resolution tunneling asymmetry scanning tunneling microscopy focusing on the locations of electrons, which will help, for example, to unlock the atomic-scale gridlock within copper oxide electronic transport system and to better understand the high temperature superconductivity.
- Using the state-of-art local probes, combining electron microscopy and scanning tunneling microscopy, the cooperative action of electron and lattice and the formation of a ferroelectric state in doped manganites were analyzed, which established the connection between colossal resistance effects and multiferroci properties, i.e., the coexistence of ferroelectric and antiferromagnetic ordering.
- A combination of first-principle theoretical calculations and atomic-resolution electron microscopy techniques provided a new understanding of the role of impurities in superconducting material, which indicates controlled impurities could further enhance the superconductivity of practical superconductors.

- The successful correction of electron microscope lens aberrations had 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.
- 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 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.
- 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.
- Developed the "Embedded Atom Method" that revolutionized the field of computational materials science by permitting large-scale simulations of atomic structure and evolution. It has been 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 nation's long-term energy strategy presents many fundamental materials challenges, especially the need for new materials and new tools to characterize them such as electron beams and scanning probes. Materials for power generation, energy storage and transportation, renewable energy, and catalysis are all affected by the structure, trace amount of specific elements and the presence of specific crystal defects. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g., defects, dislocations, grain boundaries, interfaces, magnetic domain walls, and precipitates) determine and control critical properties 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 processes on the surface and interior of nanostructures and the functionality of nanomaterials can be imaged and analyzed by using i*n-situ* microscopy techniques under various environments. The program is also relevant to the DOE energy initiatives through the local property determination of nanostructured materials for hydrogen storage and solar hydrogen generation, and structural materials for nuclear energy applications.

Scientific Challenges:

Major scientific challenges in the Electron and Scanning Probe Microscopies program are: quantitative analysis of nanoscaled structures in nanomaterials, including the atomic, electronic, and magnetic structures; fundamental understanding of scattering phenomena of charged particles in matter; understanding the atomic or nanoscale origin of macroscopic properties to enable the design of high-performance materials; imaging structure and functionality at the atomic or nanometer scale; understanding correlation between electrons and spins at the nanoscale and spin structure, dynamics, and transport properties; determination of interface structures between dissimilar materials and understanding the link between interface/surface/defect structures and materials properties; understanding the role played by individual atoms, point defects, and dopant in materials; understanding surface reactions at the atomic level in real space and imaging site specific reactivity; combination of electron and scanning probes to study complex properties; probing the local properties of materials at the atomic scale with in-situ microscopy in extreme energy environments; understanding of the structure and dynamics of ordered and disordered materials, especially the short- and long-range order effects; development of time-resolved microscopy with high resolution both spatially and temporally to study the atomic level mechanisms during structural transformations; and the application of first principles theory to understand and predict the structures and properties of real materials. To address these challenges, new state-of-the-art experimental and theoretical techniques will need to be developed. The long term goal is to develop multiscale characterization tools for linking structural evolution, dynamics, and electronic behavior with first principles understanding of materials.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
23,021	23,020	34,496

Performer	Funding Percentage
DOE Laboratories	69%
Universities	31%

*Based on FY2007
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:

This activity evolved from the program previously known as Structure and Composition of Materials and was formally renamed as Electron and Scanning Probe Microscopies in July 2007. This program will build upon the tremendous advancements in electron and scanning probe microscopy capabilities in the last decade and use scattering, imaging, and spectroscopy methods to understand functionality and fundamental processes at the atomic or nanometer scale. 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 fundamental understanding of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron and scanning probe microscopy techniques will be continued in order to meet the basic science challenges, which will be partnered with the BES Electron-Beam Microcharacterization Centers and Nanoscale Science Research Centers. The enormous improvement in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of atomic-scale tomography, probing a single electron spin and its quantum dynamics, imaging spin density in multiple dimensions, single-atom spectroscopic detection and identification, combination of multiple probes, and 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 fundamental understanding of the mechanisms by which electrons, individual atoms, surface/interfaces, and defects influence the properties and behavior of materials.

Research Activity: **Experimental Program to Stimulate Competitive Research (EPSCoR)**
Division: Materials Sciences and Engineering
Primary Contact: Tim Fitzsimmons (Tim.Fitzsimmons@science.doe.gov; 301-903-9830)
Team Leader: Helen Kerch
Division Director: Aravinda Kini, Acting

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 workforce 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 DOE 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 workforce 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.

<u>Basic Energy Sciences</u>

- Palladium complexes are among the most powerful and versatile catalysts for a variety of chemical reactions including the delivery and release of hydrogen, the chemical transformations of hydrocarbons, and the production of pharmaceuticals and industrial chemicals. Knowledge of the fundamental steps involved in these reactions is vital for the design and improvement of these important processes. Studies of these steps using both fast laser spectroscopy (taking a snapshot of the reaction) and low temperature methods (freezing the reaction midstream) have led researchers to the identification of a number of new palladium species with very short lifetimes. These species are chemically important because of their exceptionally high reactivity. Investigation of these species are leading to the production of new and more efficient catalysts for chemical processes important to energy as well as other sectors of our economy (M.J. Fink, Tulane University). Together with researchers and tools at Brookhaven National Laboratory, investigators in Louisiana are taking snapshots of catalysis processes to reveal new palladium species.

- An ever-increasing demand for portable electronic devices is driving technological improvements in rechargeable solid-state batteries. Lithium-ion batteries, with their high energy density and design flexibility, are the systems of choice. They are lightweight and have longer lifespans than other batteries. Current research in this area is aimed towards achieving higher capacity, better cycleability, and reduced “fading” by synthesizing new materials and improving existing ones. Researchers at the University of Puerto Rico are taking a new approach of replacing the liquid electrolyte with flexible polymer electrolytes in order to increase the energy density of the Li-ion batteries, looking for suitable conductivities (better than 10^{-3} S/cm) for practical energy applications. By synthesizing novel nanoparticles in polymer salt complexes, they are investigating fundamental crystalline dynamics that are leading to improved control of ion transport in these novel polymer electrolyte systems. Together with researchers from Argonne National Laboratory, their theoretical predictions of the structure and physical properties of the electrodes and electrolyte materials are being used to guide the development and synthesis of high performance materials for these applications (R. K. Katiyar, U. Puerto Rico).
- Photovoltaic devices are the most direct ways to convert solar energy to electricity. At present, photovoltaic devices based on inorganic semiconductors are efficient, but the high cost of manufacturing silicon-based devices makes the cost per watt too high to be competitive with fossil fuels. Novel photovoltaic devices based on organic, carbon-based nanostructures offer the possibility of developing low cost, easily processed thin films of polymeric materials which function as photovoltaic cells. Such devices could be competitive with other sources of energy if power efficiencies even as low as 10% can be attained. Investigators at Oklahoma State University are using first-principle, theoretical studies to investigate the electronic and structural properties of relevant conjugated polymers and carbon nanotubes. Such studies are facilitating the design and fabrication of new carbon-based materials for use in photovoltaic devices and improved renewable energy source devices (J. W. Mintmire, Oklahoma State University).
- Thermal energy exists in many forms ranging from solar energy to waste heat from existing power sources. For example, over 70% of the input power into an automobile engine is lost, a large majority of the loss in the form of waste heat. One way to harness thermal energy is through the use of thermoelectric materials and devices that enable us to transform this thermal energy into usable high quality electrical energy. Research in current thermoelectric materials is attempting to significantly increasing their efficiency. Over the past decade, significant advances have been achieved in low dimensional structures such as superlattices and quantum dots. New investigations by researchers in South Carolina using novel nanostructures and nanocomposites including exotic “cage structure” materials consist of matrices of bulk and nanomaterials are offering to nearly double the performance of low-dimensional materials. Such improved performance and continued development of high efficiency thermoelectric nanocomposites may provide environmentally safe and reliable power sources to sustain the nation’s future (T. M. Tritt, Clemson University).

<u>Biological and Environmental Research</u>

Most doses of radiation exposures associated with human activity are predicted low dose in nature. These may arise from medical diagnostics, hazardous waste abatement, power systems operation, and even terrorist acts such as dirty bombs. While the precise risk of exposure continues to be debated, recent findings indicate that a measurable risk exists even at very low doses. By measuring gene activity before and after exposure, researchers in Tennessee are working to identify biological pathways that are activated or repressed in response to the radiation insult. Work at the University of Tennessee on in situ gene expression is enhancing our understanding of low dose radiation’s effects at all levels of biological organization, from genes to cells to tissues and finally to complex organisms such as humans. Understanding the risks to human health associated with low dose radiation is critical if we are to protect the nation’s workforce while making the most effective use of national resources (M. A. Langston, U. Tennessee).

<u>Advanced Scientific Computing Research</u>

High performance anisotropic diffusion equation solver: Members of this project have [who? at what institutions?] 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 $bg \rightarrow b\phi 0$ 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 $pp \rightarrow \phi 0 \rightarrow \mu+\mu- +X$. The muon discovery channel will provide a good opportunity for a precise reconstruction of the Higgs boson masses.
- Another group at the University of Oklahoma is in the race to measure the electric dipole moment of the electron. Approximately 20 groups world wide are seeking to measure this important fundamental property that will allow the world to assign a size to the electron. Current experimental limits already show that the ratio of size of an electron to the size of a proton is less than the ratio of the size of an ant to the distance between the Earth and Sun. Specifically, the size of the electron differentiates between many competing models of how particles interact. These models include the venerable Standard Model of Physics and the newer Super Symmetric Theories. Using a lead fluoride molecule researchers at the University of Oklahoma are helping to differentiate these models (N. Shafer-Ray, U. Oklahoma).

Nuclear Energy

Gas-cooled fast reactors have the potential to use a wide range of fuel including recycled, spent nuclear fuel. Because of their high temperature operation, gas-cooled fast reactors can be used for the future production of hydrogen to replace fossil fuels for transportation. Key to the realization of the gas-cooled fast reactor is the development of a robust fuel. This fuel form must accommodate a wide variety of elements including, those in recycled fuels, and must also perform safely at very high temperatures. Researchers at the University of South Carolina are developing a composite fuel system consisting of uranium carbide microspheres contained in a zirconium carbide matrix for potential use in these reactors. This work on these fuels contributes to the safety, sustainability, and security of our energy supply for both electricity and transportation. As an additional environmental plus, use of such fuels in nuclear reactors would provide safe energy without the production of greenhouse gases (T. W. Knight, U. South Carolina).

Nuclear Physics

Magneto-inertial fusion (MIF) is an advanced form of fusion which holds the promise for safe, clean, affordable energy for the 21st century. It combines the favorable attributes of other fusion concepts currently supported by the U.S. Department of Energy, and has recently been shown to be the most economically viable way of using fusion energy for production of electricity. The University of Alabama in Huntsville is collaborating with Los Alamos National Laboratory and other institutions around the country to model the physical processes involved in MIF so that we may understand how to build a working reactor. The Huntsville group has verified that a new, advanced modeling technique called smooth particle hydrodynamics can accurately capture the physics of converging and reflecting shock waves, which is necessary for reaching fusion ignition temperatures and densities. This modeling is an important step along the road to a sustainable energy source that has the potential to liberate the United States, and the world, from its dependence on fossil fuels. Further, fusion reactors are free from many of the objectionable aspects of current nuclear power reactors and offer a more environmentally friendly alternative (J. Cassibry, U. Alabama Huntsville).

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.

<u>Defense Programs</u>
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.

<u>Fossil Energy</u>

- Fuel cells offer the promise of increasing the net efficiency of central electric coal generation plants from the present level of 30% to 35% (for conventional coal combustion systems) to levels approaching 60% to 70% (in advanced gasification systems using fuel cell, gas turbine, and steam turbine generation cycles). This increased efficiency and the attendant reduction in carbon emissions require the development of high temperature fuel cells which operate on “synthesis” gas generated from coal. However, one difficulty in using syngas in fuel cells is that it contains undesirable species such as arsenic, mercury, and nickel. A group of researchers at West Virginia University is focused on improving the reliability and life expectancy of solid oxide fuel cells in the presence of these trace contaminants. They are using atomic scale computational models to guide the development of new anode materials and macro scale modeling to predict the performance of integrated system designs for coal syngas. Industrial team members provide technical support and ensure that these results will actually be transferred to the electric power generation industry (R. Bajura, West Virginia University).
- Coal has a wide variety of trace elements such as arsenic, selenium and antimony that can have undesirable environmental consequences. In order to mitigate this potential hazard, it is important to develop a fundamental understanding of how these trace elements are partitioned in the combustion products between the gas phase and particulate matter. To correctly predict how this partitioning occurs, the generation of currently unavailable thermodynamic and kinetic data is required. Researchers in North Dakota are performing novel experiments to generate this data for these hazardous trace elements as well as for major elements, such as calcium, iron, and aluminum, over melts that replicate the solid surfaces of ash particles. Computational calculations have also been performed to compare the thermodynamic stabilities of compounds of these trace elements. Ab initio calculations suggest that oxygen-rich compounds of the trace elements are preferred to the simple oxide forms predicted by classical thermodynamic calculations. Such results are helping researchers envision the reduction of the environmental impact of burning coal (W. Seames, U. North Dakota).

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 DOE 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 2007	FY 2008	FY 2009
Alabama	393	264	0
Alaska	0	0	0
Arkansas	139	0	0
Delaware	629	980	980
Hawaii	0	0	0
Idaho	400	400	400
Kansas	0	0	0
Kentucky	450	650	650
Louisiana	440	440	440
Maine	450	650	650
Mississippi	0	0	0
Montana	134	131	0
Nebraska	269	140	0
Nevada	455	468	0
New Hampshire*	498	545	569
New Mexico	0	0	0
North Dakota	350	350	0
Oklahoma	713	661	681
Puerto Rico	0	0	0
Rhode Island	0	0	0
South Carolina	939	910	785
South Dakota	0	0	0
Tennessee**	275	275	135
Vermont	0	0	0
US Virgin Islands	-	-	0
West Virginia	495	495	0
Wyoming	140	0	0
Technical Support	111	0	110
Other***	0	7,321	2,840
Total	7,280	14,680	8,240

*Became eligible in FY2006.
**Became ineligible in April 2006. Amounts shown represent continuation funds.
***Uncommitted funds in FY 2008 and FY 2009 will be competed among all EPSCoR states.

SBIR contribution is not included in the Funding Summary Total above.

	FY 2007	FY 2008	FY 2009
SBIR	321	222	222

Projected Evolution:

A solicitation for Implementation awards was issued in FY 2007 with a due date for formal application in January 2008. A solicitation for Laboratory-State Partnership awards was issued in April 2007, and 197 pre-applications were received. Of these, 80 were invited for full proposal. Proposals were peer reviewed, and 12 University/ National Laboratory pairs selected in April 2008 for negotiation of final awards. The program continues to meet the challenge of providing a balance between the Implementation awards and the Laboratory-State Partnership awards.

Research Activity: Synthesis and Processing Science

Division:	Materials Sciences and Engineering
Primary Contact:	Bonnie Gersten (Bonnie.Gersten@science.doe.gov; 301-903-0002)
Team Lead:	Aravinda Kini
Division Director:	Aravinda Kini, Acting

Portfolio Description:

The Synthesis and Processing Science Core Research activity develops atomic- to nano-scale scientific understanding using physical principles to enable reliable, reproducible and innovative production of novel materials. This knowledge is developed through research efforts conducted in a safe and environmentally responsible manner that: (1) further our *fundamental understanding of atomistic behavior* for predictive rational design of complex (spatially and dissimilar) materials with controlled defects and architectures ranging from the atomic and molecular scales to the continuum scale; (2) revolutionize reproducible physical *synthesis strategies or techniques* (principally using bottom-up approaches) and creative processing paradigm shifts; and (3) develop *diagnostic tools* to probe synthesis, *in situ* and in real-time, with multi-technique probes that push the limits of both spatial and temporal resolutions.

Synthesis of novel materials is not limited to the atomic scale but also includes nanoscale construction of novel metamaterials, as well as complex and frustrated materials. The physical processes that are used for the synthesis of bulk crystals and thin films may include self assembly, directed assembly, layer by layer deposition, atomic probe 3-D assembly, directed or templated growth, parallel printing, nanoscale rapid prototyping, nanolithography, electrodeposition, ion beam irradiation, vapor deposition, sputtering, laser deposition, molecular beam epitaxy, pattern formation, rapid solidification, microwave synthesis or sintering. In general the program supports research efforts that advance molecular level understanding of processes based on thermodynamics, kinetics, and mechanisms, in particular nucleation and crystal growth, solidification/vitrification/devitrification, and interphases and interfaces. In addition, we seek scientific enablers to the development of new tools for synthesis of materials using a cadre of physical principles including those developed under extreme conditions of temperature, pressure, electric/magnetic field, and radiation whether under equilibrium or non-equilibrium conditions.

Unique Aspects:

Basic research supported in this activity underpins many energy related technology areas. A focus of this activity is on the exploration of physical principles and concepts in synthesizing and processing new materials that is complementary to the emphasis on: (1) chemical synthesis and chemical control of material properties in the Materials Chemistry activity and (2) biomimetic/bioinspired design and synthesis in the Biomolecular Materials activity. Significant interactions and collaborations exist between the investigators in this program and the other BES research activities, e.g., 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, and the Electron and Scanning Probe Microscopies activity for the high resolution characterization of atomic scale structure at BES supported microscopy facilities. Many of the scientists performing work on nano-materials sponsored by this activity are also leaders of corresponding science thrust areas at the BES Nanoscale Science Research Centers.

The program supports projects in research areas that are relevant to synthesis and processing science such as ion beam irradiation, molecular beam epitaxy, pulsed laser deposition and metal organic chemical vapor deposition, thermochemistry, nucleation and growth kinetics of nanorods and nanotubes, controlled nanoparticle morphology, polymer structure morphology, thin films as substrates for quantum dots and for preparing nanostructures, thin film growth for complex interfaces and superlattice growth, single crystals growth of novel materials, modeling of metallurgical processes, and colloidal assembly. In addition, the program supports the Materials Preparation Center (MPC) at the Ames Laboratory which has responded to 4,100 requests for preparation, fabrication and purification, and characterization of materials placed by customers worldwide as of FY 2007.

Relationship to Other Programs:

The Synthesis and Processing program is a critical element of the materials sciences that has emphasis in the physical sciences. This connection results in especially active interactions.

- This research activity participates in DOE's Energy Materials Coordinating Committee (EMaCC). EMaCC is a forum for information exchange and coordination with representatives from 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).
- This research activity holds joint programmatic workshops and joint solicitation panel reviews and contractor review meetings with other divisions within BES and other DOE offices. For example, the Workshop on Basic Research Needs for Materials under Extreme Environments (June 2007) involved the coordination with NNSA, FE, EERE as well as participation from many national and international laboratories, universities, and companies. Another example was the Hydrogen Program Annual Review (May 2007) held jointly with the programs within BES and EERE.
- The program also participates in the interagency coordination groups such as the NSTC MatTec Communications Group on Metals, MatTec Communications group on Structural Ceramics, and National Nanotechnology Initiative.

Significant Accomplishments:

This program is responsible for the unprecedented defect controlled thin-film growth of superconducting oxide by MBE which has allowed the discovery of photo-induced phase transitions in the films. It is also noteworthy for the mechanistic understanding of spontaneous formation of sputter ripple patterns by low energy ion beam bombardment. It has accomplished the synthesis of artificially structured thin-film semiconductors that has enabled the design of thin-film structures with desired opto-electronic properties and devices. And of significance is the accomplishment of novel processing of silicon nanomembrane on insulator which has proven that even the thinnest silicon membrane can be conductive provided the proper surface is present.

Mission Relevance:

The research in this portfolio, in support of the scientific discovery, scientific innovation, and energy security missions of the U.S. Department of Energy, not only underpins the fundamental science of synthesis and processing in general but also underpins many of the use-inspired energy-related technologies. These include the challenge of finding new superconductors, designed solid state lighting architectures and materials, catalysts, novel hydrogen storage materials, and electrical energy storage materials, photovoltaics, electrochromics, supercapacitors, fuel cells, and materials that can withstand or be prepared by extreme environments. Many of our Basic Research Needs Workshops sponsored by DOE-BES brought out a common theme of the scientific needs in materials synthesis and processing for these technologies.

Scientific Challenges:

With recent developments toward precision, in-situ, dynamic, real-time ultra-fast and ultra-small characterization equipment, and increased accessibility of computational resources, synthesis and processing has been transformed to a science with a higher level of understanding. The time is ripe to attempt to answer the many challenges presently open in this field.

- *Precision Processing:* Often precision processing comes at a cost of time and expense and is small scale. Envision what scientific approach will lead stochastic non-equilibrium processing of materials to be predictable, reliable, and uniform over large scales? Can this process be used to control defects? Can we tailor the number and distribution of defects?
- *Long and Short Range Forces*: How may we better understand long and short range forces and their contributions to the growth of nanoscale objects and of nanoscale morphology development? What are the relative roles of electrostatics and electrodynamics, and how do we relate them to the polar and acid/base approaches of the chemistry community? What are the roles of defects and long-range interactions on phase stability and interface motion?

- *Atomistic Deposition*: Atomistically controlled oxide films deposition and growth continues to provide excitement to the synthesis and condensed matter communities. Continuing unanswered questions in the synthesis of oxides include better control of deposition at low and high rates, better control of oxygen at high activities and in situ characterization improvements. As interesting as these problems are, and as interesting as the emergent behaviors they can reveal, there is the consideration of what opportunities are beyond the oxides? What is the scientific case for investigating other systems? What synthesis techniques need further development in order to have atomistically controlled deposition in these other systems?
- *Synthetic Strategies:* Even if we only consider the elements on the periodic table (and exclude the materials structure, architecture, and unnatural elements) only a small fraction of possible compounds have been synthesized. What new processing strategies can we employ that are feasible to discover new classes of materials?
- *Designing Interfaces:* What are the design rules for integrating soft with hard materials creating hybrid and dissimilar materials? Can we use synthetic techniques to create hard materials that are tailorable and soft materials that are robust? How do we synthesize soft/hard/hybrid materials that can hierarchically organize by self or through external stimuli? Can we control the 3-D architecture of these materials? Can we control the materials interfaces of heterostructures?
- *Theory:* Theory, modeling, and simulation can often complement experimental efforts, predict trends, and provide design criteria for new materials and guide experiments beyond Edisonian or "Cook and Look" approaches. Can we reverse design by proposing a desired band structure and compute the thermodynamically most plausible synthetic route? What other scientific approaches can we take?

Finally, we refer you to the challenges reported in the Basic Research Needs workshop reports and the BESAC Grand Challenge report *"Directing Matter and Energy: Five Challenges for Science and the Imagination"* for more discussion on these and other challenges.

Funding Summary:

Dollars in Thousands		
FY 2007	**FY 2008**	**FY 2009**
15,592	**16,590**	**25,529**

Perfomer	Funding Percentages*
DOE Laboratories	55%
Universities	45%

*Based on FY2007

Projected Evolution:

Over the past few years the program has evolved with an increasing interest in understanding nanoscale morphology through nucleation and growth kinetics and mechanisms, defect control in deposition processes, and complex chemical and structural materials growth. Over the next several years we expect to continue in these areas of interest, but with the added interest in the fundamental understanding of the mechanisms of interfacing soft-hard hybrid materials and the organization of these structures. We will expand our program towards the discovery of novel synthesis methods especially using extreme environments of field and flux and push the limits in our basic understanding in synthesis and processing of use-inspired technologies including solid-state lighting, solar energy conversion, hydrogen storage, and electrical energy storage.

This program will continue to support hypothesis driven fundamental science in the core research area of synthesis and processing with a particular interest in high-risk, high impact, innovative, and imaginative projects. The program continues to support and encourages natural collaboration between theorists and experimentalists to address the opportunities described in the "Scientific Challenges" above.

Research Activity: Materials Chemistry

Division: Materials Sciences and Engineering
Primary Contacts: Richard D. Kelley (Richard.Kelley@science.doe.gov; 301-903-6051)
Team Leader: Aravinda Kini
Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research in the development of novel materials and material constructs with an emphasis on synthetic 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, and molecular level understanding of friction, adhesion, and lubrication, and (5) development of new, science-driven, laboratory-based analytical tools and techniques.

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, where the emphasis is on physical control of structure and properties. Significant interactions and collaborations exist between the principal investigators in this activity and the X-Ray and Neutron Scattering activities 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 nanoscience, solid state NMR and MRI, organic magnets, organic conductors and superconductors, polymer composites, organic-inorganic hybrid 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, neutron reflectometers, combinatorial materials chemistry for new materials discovery, the surface force apparatus, and spin-polarized metastable helium scattering. 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, and engineering. This interfacing results in very active relationships.

- Within BES, there are jointly funded programs in the DOE national laboratories and universities, 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).
- Principal investigators are co-located and occasionally co-funded by EERE (batteries and fuel cells, green chemistry, solar energy conversion, and hydrogen storage), FE (catalytic materials 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 NSTC Nanoscale Science, Engineering, and Technology subcommittee (NSET), which formulated the National Nanotechnology Initiative (NNI). This subcommittee meets monthly to coordinate the NNI.
- Very active interactions with the National Science Foundation (NSF) through joint workshops and joint funding

of select activities as appropriate (two currently active).

Significant Accomplishments:

This activity is responsible for the discovery of the first organic magnet, the highest-T_c organic superconductor, the first all-organic superconductor, and the first room temperature organic magnet. 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. The first material that simultaneously exhibits bistability in three physical channels – electronic, magnetic, and optical – was discovered. 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. New combined experimental and theoretical work has demonstrated that semiconductor nanowires can be designed to achieve extremely large enhancements in thermoelectric efficiency, a factor of 100 for silicon, and that the temperature of maximum efficiency may be tuned by changing the dopant and the nanowire size. Theory indicates that similar improvements should be achievable for other semiconductor systems because of phonon effects. Another nanoscience accomplishment involves the discovery of a new, inherently inexpensive solution-based technique to synthesize one-dimensional “superlatticed” nanorods. Superlatticed refers to semiconductor structures with alternating layers of different compositions. Theoreticians in the multi-investigator group who achieved this predicted that as the composition of the superlattice was changed strain engineering would induce the spontaneous formation of one-dimensional materials and superlatticed structures with their predicted outstanding electronic and photonic properties playing a key role in devices.

This activity 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. This activity 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. Recent work by this group is the first application of gas phase MRI to microfluidic catalysis. They developed a technique in which parahydrogen-polarized gas is used to make an MRI signal strong enough to provide direct visualization of the gas-phase flow over active catalysts in packed-bed microreactors. These early results are expected to have significant effects on catalysis research in the near future.

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. The Materials Chemistry 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 materials characterization. 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. Realization of this challenge can lead to novel synthesis routes to new materials and new materials properties.

Funding Summary*:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
46,439	43,430	61,310

.

Performers (FY2005)	Funding Percentage**
DOE Laboratories	49%
Universities	51%

* Represents combined total for Materials Chemistry and Biomolecular Materials.
**Based on FY2007
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, with an emphasis on the discovery of new materials and strategies for solar energy conversion, hydrogen generation and storage, and electrical energy storage. It will seek to develop new multi-disciplinary approaches, with 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 also include novel materials and innovative concepts that will impact electrical energy storage, novel electrodes and membranes for improving the efficiency of fuel cells, and theory and modeling to aid new materials discovery. Also of interest is the development of new instrumentation to measure forces and other physical and chemical properties with ultrahigh sensitivity to further advance the nanoscale science. 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 strive to identify and support high-risk, high-impact, and often ground-breaking research.

Research Activity: Biomolecular Materials

Division: Materials Sciences and Engineering
Primary Contacts: Aravinda Kini (Arivinda.Kini@science.doe.gov; 301-903-3565)
Team Leader: Aravinda Kini
Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports fundamental research in the design and synthesis of novel materials and material assemblies by using concepts and principles of biology. The major programmatic emphasis is on exploring molecules and processes of the biological world that could be utilized or mimicked in designing novel materials, processes, and devices with potential energy significance in support of DOE's mission. Major thrust areas include:
(1) understanding, controlling, and building complex structures by self-, directed- and hierarchical assembly, the approach widely found in Nature; (2) biomimetic and/or bioinspired routes to synthesize energy relevant materials, e.g., semiconductor, ferroelectric, optical, and magnetic materials; (3) design and synthesis of functional materials and complex structures with properties and capabilities found in Nature, e.g., emergent behavior, self-repair;
(4) design and synthesis of multi-component, e.g., inorganic, organic, polymeric and biological, materials that will develop new functions and collective properties that are not achievable in individual components alone;
(5) materials aspects of biological energy conversion and storage; and (6) development of science-driven "Tools and Techniques" for the characterization of biomolecular and soft materials.

Unique Aspects:

Basic research supported in this activity underpins many energy-related technological areas such as energy conversion and storage, light-weight and high-strength materials, efficient membranes for highly selective separations, and advanced catalytic systems/architectures similar to natural enzymes with high specificities and high turnover ratios. Focus of this activity on the exploitation of biology in the quest for new materials is complementary to the emphasis on: (1) exploratory chemical synthesis of materials and chemical control of properties in the Materials Chemistry activity; and (2) physical principles and concepts such as nucleation, diffusion, solidification, and phase transformations in the Synthesis and Processing Science activity. Similarly, the Biomolecular Materials activity, with its principal interests in areas at the intersection of biology and materials sciences, complements the Energy Biosciences activity in the Chemical Sciences, Geosciences and Biosciences Division, whose focus is on areas where biological sciences intersect with energy-relevant chemical sciences. Significant interactions and collaborations exist between the principal investigators in this activity and other core research activities, e.g., with 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 work at the bio/nano interface sponsored by this activity are also leaders of corresponding science thrust areas at the BES Nanoscale Science Research Centers supported by the Scientific User Facilities Division.

To a large measure, the scientific thrusts pursued in this portfolio are multi-investigator and multi-disciplinary type as they require strong interactions between the physical sciences and life sciences. Investigators supported in this program are world leaders in biomolecular materials, encompassing topics such as self- and directed assembly, interfacial science, bio-nanoscience, hybrid (organic-inorganic-biological) materials, phospholipid membrane biophysics, and bioinspired materials and concepts in friction, adhesion, and lubrication. Several investigators in this program are pioneers of novel synthetic strategies such as the use of biomolecules as catalysts and/or templates for materials synthesis, combinatorial chemistry for new materials discovery, generation of a bacterium with unnatural amino acid genetic code, bio-inspired polymer architectures that self-assemble into pre-designed macroscopic structures, DNA-directed assembly of nanocrystals, and development of novel tools and techniques to probe biomolecular materials and processes. The activity has sought to maintain an optimal balance between "discovery-class research" and "use-inspired basic research," and will continue to identify and support high-risk, high-impact research that can potentially result in ground-breaking discoveries.

Relationship to Other Programs:

The Biomolecular Materials program is a vital component of the materials sciences that interfaces materials sciences with biology. This interfacing results in very active relationships.

- 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).
- Within BES, there are jointly funded programs between the DOE national laboratories and universities (about six currently), joint program reviews, joint contractor meetings (with EERE), and workshops.
- The program coordinates through the NSTC Nanoscale Science, Engineering, and Technology subcommittee (NSET), which formulated the National Nanotechnology Initiative (NNI). The NSET subcommittee coordinates the NNI among a large number of federal agencies.
- Very active interactions with the National Science Foundation (NSF) and National Institutes of Health (NIH) through joint workshops and joint support of National Academy studies in relevant areas (two currently active).

Significant Accomplishments:

This program is responsible for pioneering the combinatorial materials synthesis approach for the discovery of new inorganic materials. Combinatorial chemistry was previously developed for high-throughput synthesis of a library of biologically active molecules to assist in drug discovery. Biosynthetic routes found in Nature (e.g., in marine sponges, magnetotactic bacteria) have been harnessed to produce a wide variety of semiconductor, ferroelectric, and magnetic nanocrystals under mild conditions and under environmentally benign conditions. Another remarkable achievement is the development of a method to genetically encode unnatural amino acids (beyond the common twenty) with diverse physical, chemical, or biological properties in bacteria *E.Coli* and mammalian cells. The expanded amino acid genetic code makes it possible to synthesize proteins incorporating unnatural amino acids, thereby producing “synthetic” analogs of proteins. This can eventually lead to our ability to generate entirely new functional biomolecular materials, and even make it possible to go beyond proteins to prepare the long-sought-after mono-disperse versions of industrial polymers such as polyesters and polyimides. A novel strategy to stabilize liposomes as well as to immobilize them on surfaces has been demonstrated by use of nanoparticles. This strategy addresses the longstanding challenge of enhancing the stability and durability of phospholipid bilayer structures so that they can be used in materials applications as smart materials, nanoscale chemical reactors for massively parallel synthesis, etc. Integrating carbon nanotubes with proteins and living cells has recently been accomplished by use of synthetic polymers appended with sugar molecules, and surprisingly, the hybrid composite (nanotube-polymer-sugar molecule) was found to be non-toxic to cells. Nanotube-living cell hybrid structures combine the biological functions of cells with electronic and optical properties of nanotubes as a model multi-functional, biomolecular material construct. A broad-spectrum light-harvesting system that self-assembles into precisely shaped rods like tobacco mosaic virus and mimics the antenna in photosynthetic bacteria has been developed. Recently, the DNA-guided assembly of nanoparticles into three-dimensional crystalline assemblies has been demonstrated for the first time.

Mission Relevance:

The research supported in this activity addresses many of DOE’s strategic themes including Energy Security, Scientific Discovery and Innovation, and Environmental Responsibility. The research in this portfolio underpins many energy-related technological areas such as catalysis; energy conversion and storage; friction, adhesion, and lubrication; hydrogen generation and storage; light-weight high-strength materials; and membranes for advanced separations.

Scientific Challenges:

The major scientific challenges that drive the Biomolecular Materials activity directly correspond to four out of the five scientific grand challenges in basic energy sciences, as described in the report, *Directing Matter and Energy: Five Challenges for Science and Imagination.* The four grand challenges are: (1) How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties? (2) How do remarkable properties of matter emerge from complex correlations of the atomic and electronic constituents and how can we control these properties? (3) How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems? And, (4) how do we characterize and control matter--especially very far away--from equilibrium? Since biology has already figured out, albeit over several billion years, ways in which matter, energy, entropy, and information are organized and/or manipulated, the challenges for us is to understand, adapt, and improve upon them so that it will become valuable and practical under a broader range of non-biological and harsher conditions.

Funding Summary*:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
46,439	43,430	61,310

Performers (FY2005)	Funding Percentage**
DOE Laboratories	49%
Universities	51%

*Represents the combined totals for Materials Chemistry and Biomolecular Materials.
**Based on FY2007
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:

This activity will strive to maintain a well-balanced research portfolio that addresses both "discovery-oriented" and "use-inspired" basic science. It will also seek to support high-risk scientific pursuits that are curiosity-driven, and develop new multi-disciplinary approaches, with biology, chemistry, physics, and computational science playing major roles, to model, design, and synthesize novel materials with unique functionalities. The program will continue to seek a fundamental understanding of thermodynamic, kinetic, and dynamical aspects of "self-assembly" to produce both equilibrium and non-equilibrium material structures. In addition to the current thrust areas mentioned above, the program will expand in the following areas: self-healing and self-repairing materials; effective strategies for interfacing biological and non-biological materials systems in search of multi-functional materials and emergent behavior; synthetic enzymes; material architectures for efficiently integrating light-harvesting, photo-redox, and catalytic functions to convert carbon dioxide into liquid fuels; and biomolecular functional devices that take inspiration from biological gates, pores, channels, and motors.

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)
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 Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL); 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 the most powerful short-pulse spallation neutron source in existence. 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 short 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 9,000 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 objectives are 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 8,500 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, other agencies, industry, and 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, has 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 defects in automotive gears and brake discs and 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.

Scientific Challenges:

The synchrotron radiation light sources. First, the beginning of top-off operations at SSRL and ALS requires installation of interlock systems and beamline apertures. This mode of operation will significantly increase the average x-ray source intensity and brightness. 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, optimal utilization of the LCLS coherent short-wavelength x-ray source will require successful fabrication, installation, and commissioning of advanced instruments.

The neutron scattering sources. First, new instrumentation at HFIR must be successfully integrated into a robust user program. Second, the SNS must successfully perform its early operational phases.

Funding Summary:

Dollars in Thousands

	FY 2007	FY 2008	FY 2009 Request
Advanced Light Source	48,797	47,367	51,049
Advanced Photon Source	105,000	105,000	116,514
National Synchrotron Light Source	36,900	36,900	40,149
Stanford Synchrotron Radiation Laboratory	30,725	30,825	33,028
High Flux Isotope Reactor	55,705	54,511	58,780
Intense Pulsed Neutron Source	15,500	8,000	4,000
Manuel Lujan, Jr. Neutron Scattering Center	10,500	10,500	11,155
Spallation Neutron Source	165,500	164,640	177,640
Linac for LCLS	37,550	61,500	96,700
X-ray and Neutron Scattering Facilities, Total	506,177	519,243	589,015

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: **Nanoscale Science Research Centers**
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 the 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 major projects to construct, establish, and equip the NSRCs are now complete, with the last one finished in FY 2008; all five facilities are in full operations serving the user community. All encompass state-of-the-art instrumentation and expert staff to support the synthesis, processing, fabrication, analysis, simulation, and characterization of materials at the nanoscale. The NSRCs are major user facilities serving researchers from academia, national laboratories, and industry and already serve nearly 800 users annually.

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 make sophisticated research tools for nanoscience and nanotechnology available to the broad scientific community, and 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 programs 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 leverage the capabilities 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. While not a requirement, 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 six new buildings has been completed for the five NSRCs, the initial complement of technical equipment has been successfully installed and commissioned, and all five facilities entered full user operations between FY 2006 and FY 2008. All five 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. Hundreds of 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. In the operations phase of the NSRCs, user activity has picked up accordingly, with nearly 800 unique users in FY 2007 for the four centers that had operations funding that year. Research highlights include the DNA-mediated crystallization of nanoparticle arrays into three-dimensional ordered structures, the production of hollow protein nanotubes by self-assembly of surface-modified hexameric ring structures, and the deposition of metallic nanoparticles on a preapplied film of carbon nanotubes on plastic to create flexible hydrogen sensors.

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 numerous follow-up reports on Basic Research Needs for specific focused aspects of energy research, such as the hydrogen economy, solar energy utilization, and solid-state lighting. 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 necessary to help our nation develop a balanced research and development infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the 21st century. Nanotechnology R&D is a top federal priority with broad potential implications for the nation's competitiveness. DOE's participation in this effort includes the development and operation 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 specific scientific challenges, many of which benefit from the collocation of disparate disciplines in order to fabricate, assemble, and otherwise manipulate 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 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 2007	FY 2008	FY 2009 Request
Construction:			
The Molecular Foundry, LBNL	257	0	0
Center for Integrated Nanotechnologies, SNL/LANL	247	0	0
Center for Functional Nanomaterials, BNL	18,864	363	0
Other Project Costs - CFN	500	0	0
Operation:			
Center for Nanoscale Materials, ANL	18,019	18,526	20,857
Center for Nanophase Materials Sciences, ORNL	18,115	18,000	19,975
The Molecular Foundry, LBNL	19,056	18,250	20,150
Center for Integrated Nanotechnologies, SNL/LANL	17,864	18,100	20,100
Center for Functional Nanomaterials, BNL	0	18,250	20,150
TOTAL	92,922	91,489	101,232

Projected Program Evolution:

The NSRCs are completing the transition to standard user operations within the new facilities and with their initial suite of specialized technical equipment. This process is bringing 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 are already adapting to respond to the needs of the community, with targeted acquisitions of new capital equipment and allocation of staff and accompanying resources to those areas that are most in demand. While a substantial user base is established already, the NSRCs are still being assimilated into the national scientific infrastructure; there will continue to be an increase in submitted proposals with a corresponding increase in users and/or corresponding decrease in the proposal approval rate, until a steady state is reached. The NSRCs are expected to perform as world-leading institutions, excelling both in scientific impact and productivity and in working with users. These are the fundamental criteria for evaluation of the NSRC facilities; each has undergone an initial (baseline) operations review and subsequent reviews will follow triennially.

Research Activity: **Electron-beam Microcharacterization Centers**
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 National Center for Electron Microscopy (NCEM) at Lawrence Berkeley National Laboratory (LBNL); the Electron Microscopy Center for Materials Research (EMC) at Argonne National Laboratory (ANL); 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 other BES-funded efforts, have collaborated on the Transmission Electron Aberration-corrected Microscope (TEAM) 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, which will be sited at NCEM and available to users by the end of FY 2009.

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 TEAM instrument is capable of 0.05 nm direct spatial resolution). 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 spanned instrumental improvements in resolution and other performance measures, development of unique capabilities, and outstanding scientific results. This includes the development and operation of the Atomic Resolution Microscope (in the early 1980s) and One-Angstrom Microscope (in the late 1990s) at NCEM, followed by the multi-laboratory project to create the TEAM instrument (which will conclude in 2009); all constituted 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 advances across this suite of facilities have included detection of picometer-scale strain relaxation in magnetic nanoparticles leading to core-shell segregation and catalytic surface activity, and development of new approaches to characterize magnetic spins and other properties at higher spatial resolution than was previously possible.

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 their 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:

A wide variety of major scientific challenges that could be uniquely or most effectively addressed by electron scattering methods have been delineated in workshops on future science needs and opportunities for the field and on planning for the TEAM project. These challenges include:

- Investigating synthesis and assembly of nanomaterials
- Clarifying size effects on thermodynamic properties of nanostructures
- Direct comparison of theory and experiment at the nanoscale through the determination of the three-dimensional atomic-scale structure of nanostructures
- Determining the nanoscale origins of macroscopic properties, such as strength and conductivity, for high-performance materials ranging from those used in structural applications to those used in microelectronics
- Understanding the roles of individual atoms, point defects, and dopants in materials, such as in GaN for solid-state lighting or the role of oxygen in high-temperature superconductivity
- Characterization of interfaces in materials at arbitrary orientations, between ordered and disordered materials, and at hard/soft interfaces and phase boundaries
- Mapping of electromagnetic (EM) fields in and around nanoscale matter, including the atomic-scale origins of magnetism at the nanoscale
- Probing structures in their native environments, including atomic-scale investigation of functioning catalysts, corrosion processes, oxidation, biomaterials, and organic-inorganic interfaces
- Explaining the behavior of matter far from equilibrium, such as dynamic/transient behavior and environments involving high radiation, pressure, or temperature

Funding Summary:

Dollars in Thousands

	FY 2007	FY 2008	FY 2009 Request
Electron Beam Centers	8,040	8,183	11,250
TEAM Project	5,508	6,687	0

Projected Program Evolution:

The electron-beam characterization facilities were previously supported within BES research programs and were transitioned in FY 2007 to 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. The TEAM project has resulted in substantial advancements, including the creation of a dramatically different specimen stage configuration that offers more precise, stable, and flexible sample handling and manipulation, as well as the first implementation of chromatic aberration correction in transmission electron microscopy. The use of this instrument offers improved performance and new kinds of experiments; furthermore, there is the potential for developing additional instruments that use these platform technologies and are tailored for specific kinds of research (e.g., in-situ processing or fields, spectroscopy, etc.). Further program evolution will be driven by the scientific challenges described above and will require corresponding instrumental and technique improvements including work on in-situ environments; advanced electron, photon, and x-ray detectors; better temporal resolution; improved and specialized electron sources; electron optical configurations designed for interrogating materials under multiple excitation processes; and community software tools including virtualized instruments and improvements in remote operation.

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 such 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. To exploit fully the fluxes delivered by synchrotron radiation facilities and the Spallation Neutron Source (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 9,000 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 a 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.

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 will 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 2007	FY 2008	FY 2009 Request
1,476	1,833	9,120

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.

Research Activity: Atomic, Molecular, and Optical Science

Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact: Jeffrey L. Krause (jeff.krause@science.doe.gov; 301-903-5827)
Team Lead: Michael Casassa
Division Director: Eric A. Rohlfing

Portfolio Description:

The Atomic, Molecular, and Optical Science (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 length scale and sub-picosecond time 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 broadly enable the fundamental science efforts of the Department of Energy (DOE), including research conducted at BES user facilities. The results of this research have wide applicability in enabling science and technology. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, enhances our ability to understand materials of all kinds, and enables 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), the Advanced Photon Source (APS), the Photon Ultrafast Laser Science and Engineering (PULSE) Center, and the Ultrafast X-ray Science Laboratory (UXSL). AMOS is a major supporter of synchrotron-based AMO science in the United States, and continues its role as the principal U.S. supporter of research into the properties and interactions of atomic and molecular ions relevant to fusion plasmas.

Relationship to Other Programs:

The AMOS program supports planned experiments concerning x-ray characterization and AMO science at 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 PULSE center at SLAC, which is co-supported by the BES Materials Sciences and Engineering Division, and the UXSL at Lawrence Berkeley National Laboratory (LBNL). 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. A close working relationship exists with the National Science Foundation (NSF) Atomic, Molecular, Optical and Plasma Physics Program. These two programs co-funded 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 2007, the AMOS Program provided partial support for the Gordon conferences on Quantum Control of Light and Matter, and Atomic Physics, the conference on Fundamental Optical Processes in Semiconductors, and the Joint Conferences on Ultrafast Optics and Applications of High Field and Short Wavelength Sources. In FY 2008, the AMOS program provided partial support for the Gordon conference on Photoions, Photoionization and Photodetachment.

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, 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. This 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 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 research at 4th generation light sources such as the LCLS. X-ray pulses with durations of femtoseconds can produce stop-action pictures of the motion of atoms during molecular transformations. New sources, with pulses of attosecond duration may make it possible to image the real-time motion of the electrons during the course of chemical reactions. Recent progress has been reported in the generation of ultrashort x-ray pulses from table-top, laser-based sources that provide complementary capabilities to planned x-ray free electron lasers, such as the LCLS. In one example, hard-x-ray pulses were generated from a liquid mercury target irradiated by high power, femtosecond laser pulses. In another approach, high harmonic generation in gases has been used to shift laser light from the infrared or visible to extreme-ultraviolet or soft x-ray wavelengths. Suitable optical manipulation of the harmonics can be used to produce x-ray pulses of a few attoseconds in duration. Finally, theorists have suggested a method to use intense, ultrafast laser pulses to make a gas transparent to x-rays for the duration of the laser pulse. If realized experimentally, this device could be used as an ultrafast switch to slice a femtosecond pulse from a much longer x-ray pulse. Recognition of international scientific leadership by AMOS-sponsored investigators includes MacArthur, Rabi, Goeppert-Mayer, Davisson-Germer awards; American Physical Society Fellowships; and National Academy memberships.

Mission Relevance:

AMO science empowers 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, such as 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 effort to understand nanoscale light-matter interactions is central to research in photo-energy conversion relevant to the use of solar energy, enables the development of 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 length scale and sub-picosecond time scale. AMOS contributes at the most fundamental level to the science-based optimization of current energy sources and the development of new sources.

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 wave functions 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 that manifest novel light-matter interactions and properties; and coherently drive electrons in atoms, plasmas, or synchrotron orbits to generate ultrafast x-ray pulses. Theoretical advances are enabling modeling and simulation of increasingly complex systems to provide interpretation of existing data and predictions for new experiments. These capabilities create opportunities to investigate chemical processes under conditions that are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons. Research in AMO science is fundamental to meeting the grand challenges for basic energy sciences, as identified in the recent report on this topic from the Basic Energy Sciences Advisory Committee.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009 Request
18,112	18,112	23,659

Performer	Funding Percentage
DOE Laboratories	48 %
Universities	52 %

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 AMOS activity provides funding for 53 university grants that partially support 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 capitalize upon unique facilities at the DOE national laboratories, including the MIRF at ORNL, the ALS at LBNL, the APS at Argonne National Laboratory (ANL), and the LCLS which will be operational in 2009 at SLAC. 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 also 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 by ultrafast lasers or collisions with highly charged ions.

Projected Evolution:

The AMOS activity will continue to support 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 of molecular processes; 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 and attosecond pulses of x-rays at existing synchrotrons as well as new accelerator-based and table-top 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. Studies of 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 will continue. Fundamental studies of atomic and molecular ions and their interactions with atoms, molecules, and surfaces will further develop the knowledge base vital to understanding fusion plasmas. Experimental and theoretical AMOS tools will be used 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
Primary Contacts:	Gregory J. Fiechtner (gregory.fiechtner@science.doe.gov; 301-903-5809)
Detailees:	Wade N. Sisk, BNL (wade.sisk@science.doe.gov; 301-903-5692)
	Larry A. Rahn, SNL-CA (larry.rahn@science.doe.gov; 301-903-2508)
Team Lead:	Michael P. Casassa
Division Director:	Eric A. Rohlfing

Portfolio Description:

This activity supports experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aimed at elucidating the molecular-scale chemical and physical properties and interactions that govern reactivity, solute/solvent structure, and transport. Also supported are studies motivated by new opportunities fostered by predictive understanding of chemical reactivity, including structural and dynamical studies that emphasize a complete understanding of reactive chemistry. These activities include the development and implementation of predictive computational modeling and simulation approaches, incorporating advanced theory and experimental validation, for scientific discovery across multiple scales. Impact on DOE missions is far reaching, including energy utilization, catalytic and separation processes, energy storage, and environmental chemical and transport processes. The activity is implemented as two distinct programs: (1) Gas Phase Chemical Physics (GPCP) and (2) Condensed Phase and Interfacial Molecular Science (CPIMS).

GPCP 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 a fundamental understanding of chemical reactivity enabling validated theories, models and computational tools for predicting rates, products, and dynamics of chemical processes involved in energy utilization by combustion devices. Important to this aim is also the development of experimental tools for discovery of fundamental dynamics and processes affecting chemical reactivity.

CPIMS research emphasizes molecular understanding of chemical, physical, and electron driven processes in aqueous media and at interfaces. Studies of reaction dynamics at well-characterized metal and metal-oxide surfaces and 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 first-principles understandings of molecular reactivity and dynamical processes in solution and at interfaces. The approach confronts the transition from molecular-scale chemistry to collective phenomena in complex systems, such as the effects of solvation on chemical structure and reactivity.

Unique Aspects:

The BES Chemical Physics Research activity is unique in its long term support of a number of fundamental chemical science areas, and in its integration of capabilities from research universities and DOE national laboratories that sustain long-term progress in difficult scientific areas as well as effective coupling to DOE missions.

Through the GPCP portfolio, DOE is the principal supporter of high-temperature chemical kinetics and gas-phase chemical reaction dynamics in the nation. This activity also has oversight for several national laboratory programs, including the Combustion Research Facility (CRF), a unique facility that hosts a strong visitors program for collaborating scientists and promotes synergism between the BES-supported basic research and the applied science and technology programs supported by the Office of Fossil Energy (FE), the Office of Energy Efficiency and Renewable Energy (EERE), and industry.

The CPIMS portfolio is unique is its relevance to DOE mission areas, providing a fundamental basis for understanding chemical reactivity in complex systems, such as those encountered in catalysis, energy storage, separations, and the environmental contaminant transport in mineral and aqueous environments. This program is a major supporter of basic research on chemical reactivity of molecular species in the liquid phase, on metal clusters, and at solid-gas and solid-liquid interfaces. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiolysis effects and radiation-driven chemistry in nuclear fuel and waste environments.

Relationship to Other Programs:

Research under this activity complements research supported across the Office of Basic Energy Sciences, including Catalysis Science, Separations and Analysis, Heavy Element Chemistry, Atomic and Molecular Optical Science, Solar Photochemistry, and Geosciences. There is a particularly strong coupling between the CPIMS and Solar Photochemistry programs in the fundamental chemistry and physics of radiolytic processes in condensed media and at interfaces. There are also numerous linkages with combustion research conducted under various research programs within DOE EERE and DOE FE as well as combustion-related chemical physics research 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 the National Science Foundation (NSF). These linkages include common PIs and industry relationships in a number of programs, as well as the couplings described above fostered by the CRF. This activity provides substantial support for basic research to scientists at PNNL who utilize the William R. Riley Environmental Molecular Sciences Laboratory (EMSL), a national user facility operated by the DOE/SC Office of Biological and Environmental Research (BER).

Significant Accomplishments:

Impacts in fundamental science include the development of crossed molecular beams and ion imaging techniques that have spawned a generation of experiments in state-to-state chemical reaction dynamics and energy transfer, much of which has been supported by the chemical physics program. In addition, support from this activity resulted in the development of molecular beam and laser sputtering techniques for the study of atomic clusters as prototypical models for catalysis. More recently, ultrafast laser spectroscopy has provided important insights into hydrogen bonding and proton transport in water in nano-confined geometries. Advanced probes of combustion environments have also yielded recent discoveries, such as the direct observation of reactions important in incipient soot formation and the recent discovery of the importance of enols in flame chemistry. This activity has played a major role in the development of quantum chemistry methodologies for accurate predictions of chemical properties. These developments have led, in turn, to theories and computer codes for the calculation of thermodynamic properties and chemical reaction rates in the gas phase as well as the properties of complex molecular systems in the condensed phase.

Mission Relevance:

The GPCP portion of this activity contributes strongly to the DOE mission in the area of the efficient and clean combustion of fuels, enabling new opportunities fostered by an increasingly predictive understanding of chemical combustion. Since 85 percent of nation’s energy use is derived from burning fossil fuels, this activity is motivated by national needs in energy security, economic growth, and environmental preservation. The chemical complexity of combustion has provided an impressive challenge to predictive modeling. Truly predictive combustion models will enable the design of new combustion devices (such as internal combustion engines, burners, and turbines) with maximum energy efficiency and minimal environmental consequences. In transportation, the changing composition of fuels, from those derived from light, sweet crude oil to biofuels and fuels from alternative fossil feedstocks, puts increasing emphasis on the need for science-based design of innovative new devices.

The CPIMS portion of this activity provides fundamental underpinnings relevant to energy production and storage, along with energy-relevant processes such as chemical separations and catalysis. Surface-mediated catalysis, for example, reduces the energy demands of industrial chemical processes by bypassing energy barriers to chemical reaction. The knowledge gained from this research program will aid in the development of a predictive capability for surface chemistry. Basic research with respect to radiation-induced excited species in the condensed-phase provides fundamental knowledge relevant to solar energy production and environmental remediation. This activity also contributes to DOE missions in areas of waste remediation and radiation effects associated with nuclear energy production.

Scientific Challenges:

- Improve and expand experimental measurement of highly energetic, unstable molecules to diagnose complex reacting flows and, in more controlled environments, to determine molecular dynamics and reaction rates at elevated temperatures.

- 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 computation of properties and reactions of large molecules.
- Improve accuracy and throughput of 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, catalysis, and condensed phase processes.
- Develop fundamental understanding of the mechanisms that underlie assembly of atoms into clusters and larger nanosystems for the rational design and synthesis of cluster-based nanoarchitectures with desired properties.
- Develop and apply new experimental methods for characterizing chemically active molecular scale structures and reaction mechanisms at interfaces.
- Characterize high-energy electron- and photon-stimulated processes at complex interfaces.
- Design quantitative models for condensed-phase solvation that include polarization, charge-transfer, and nano-confinement 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 2007	FY 2008	FY 2009 Request
Chemical Physics Research (Total)	33,877	34,777	52,764

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. Beginning in FY 2009, this activity assumes oversight of the CRF operational budget of approximately $7.2M per year.

Performer	Funding Percentage
DOE Laboratories	68 %
Universities	31 %
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, energy conversion and storage, and environmental preservation. The desired evolution is to predictive capabilities that span the microscopic to macroscopic domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices. Currently, increased emphasis in gas-phase chemical physics is on validated 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 emphasis 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, emphasis 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, broaden efforts to molecular building blocks of emerging fuels, probe the chemical physics of energy transfer in large molecules, and to explore the molecular origins of condensed phase behavior and the nature and effects of non-covalent interactions including hydrogen bonding. A continuing emphasis on DOE mission impact will guide the selection of research opportunities, development of predictive capabilities, and interactions with other programs and organizations.

Research Activity: **Solar Photochemistry** (formerly Photochemistry and Radiation Research)
Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact: Mark T. Spitler (mark.spitler@science.doe.gov; 301-903-4568)
Team Lead: Richard Greene
Division Director: Eric A. Rohlfing

Portfolio Description:

This activity supports photochemical studies relevant to capture and conversion of solar energy and fundamental studies in chemical and physical properties induced by ionizing radiation. 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 sciences investigates fundamental physical and 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 as are radiolytic reactions in ionic liquids. Specialized accelerator facilities for electron pulse radiolysis are supported at Brookhaven National Laboratory (BNL) and the Notre Dame Radiation Laboratory.

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. Fundamental studies of radiation science 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.

Unique Aspects:
This activity is the dominant supporter of solar photochemistry research in the United States and provides unique support for radiation science via specialized electron pulse radiolysis facilities at Notre Dame and BNL, which serve the academic research community, industrial users, and other Department of Energy (DOE) national laboratories

Relationship to Other Programs:
The solar photochemistry research effort interfaces with several activities in BES: Photosynthetic Systems activities in biochemical aspects of photosynthesis; Chemical Physics in theoretical calculations of excited states and computational modeling; Catalysis Science in 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 the DOE Office of Energy Efficiency and Renewable Energy (EERE) activities in its Solar Energy Technologies Program on photovoltaics and its Hydrogen, Fuel Cells, and Infrastructure Technologies Program.

The radiation sciences activity is closely coordinated with the BES Condensed Phase and Interfacial Molecular Sciences in the physical and chemical aspects of radiolysis. The radiation science effort also coordinates with BES Catalysis Science in reaction kinetics in homogeneous solutions, and Mechanical Behavior and Radiation Effects in radiolytic damage to glasses and radiation-induced corrosion of structural materials. There are also important interfaces with the DOE Office of Environmental Management activities in waste remediation and Office of Nuclear Energy activities on nuclear reactors, and nuclear waste processing and storage.

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 Argonne National Laboratory (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 the National Renewable Energy Laboratory involving shared research, analytical and fabrication facilities, and a jointly shared project on dye-sensitized solar cells. 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:

The major challenges in solar photoconversion have been outlined in a recent BES workshop on “Basic Research Needs for Solar Energy Utilization.” Among these challenges, knowledge gained in charge separation and long-distance electron transfer needs to be applied in a meaningful way to activation of small molecules such as CO_2 and H_2O via photocatalytic cycles to transform them into fuels. 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 nanoparticulate solids, and the study of the mechanism of multiple exciton generation (MEG) within nanoparticles. 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. There are also challenges in fundamental understanding of photoconversion processes – energy transfer and the generation, separation, and recombination of charge carriers – in organic-based molecular semiconductors, which could lead to a new type of inexpensive and flexible solar cell. 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 “Basic Research Needs for Advanced Nuclear Energy Systems” has identified new directions, connections, and roles for radiation chemistry in the nuclear energy systems of the future. 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. 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

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009 Request
30,603	30,603	39,569

Performer	Funding Percentage
DOE Laboratories	53%
Universities	47 %

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 approximately 55 university grants supporting about 100 graduate students and postdoctoral research associates, and partially supporting about 50 faculty. There are 10 programs at DOE national laboratories supporting about 45 senior staff and 50 graduate students and postdoctoral research associates. Programs at the laboratories are multi-investigator efforts on problems that require extensive participation by senior experienced 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 DOE 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 and BNL.

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 multiexciton generating quantum dots, 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 and efficient 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. 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.

Research Activity: **Energy Biosciences Research**
Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact: Richard V. Greene (richard.greene@science.doe.gov; 301-903-6190)
Detailee: Robert Stack, PNNL (robert.stack@science.doe.gov; 301-903-5652)
Team Lead: Richard V. Greene
Division Director: Eric A. Rohlfing

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, biophysical, 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 and physical 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 control the architecture of energy transduction systems and deposition of solar energy into chemical energy storage products, inclusive of cell wall polymers, starch, lipids, etc. (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 energy and material production, as well as active site chemistry for bioinspired catalysts. (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 a unique 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 Solar Photochemistry 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 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. 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 2007	FY 2008	FY 2009 Request
Photosynthetic Systems	14,750	14,750	19,926
Physical Biosciences	14,175	14,175	15,675
Energy Biosciences Research (Total)	28,925	28,925	35,601

Performer	Funding Percentage
DOE Laboratories	16 %
Universities	79 %
Other	5 %

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 molecular biology and biochemistry with powerful capabilities in imaging and computation. This will, for example, allow 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. 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. Future impact is also envisioned through 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 catalysts.

The Energy Biosciences program will evolve into two programs in FY 2009: 1) Photosynthetic Systems (formerly named Molecular Mechanisms of Natural Solar Energy Conversion); and 2) Physical Biosciences (formerly named Metabolic Regulation of Energy Production). Both programs support fundamental research on plant and microbial systems. It is envisioned that solar energy utilization research will be particularly enhanced through complementary efforts between the Photosynthetic Systems and Solar Photochemistry programs. Similar complementation will occur between the Physical Biosciences program and the Catalysis Science and Separations & Analysis programs.

Research Activity: **Catalysis Science** (formerly Catalysis and Chemical Transformations)

Division: Chemical Sciences, Geosciences, and Biosciences

Primary Contacts: Raul Miranda (raul.miranda@science.doe.gov; 301-903-8014)
Paul H. Maupin (paul.maupin@science.doe.gov; 301-903-4355)

Detailee: Michael Chen, ANL (michael.chen@science.doe.gov; 301-903-2368)

Team Lead: John C. Miller

Division Director: Eric A. Rohlfing

Portfolio Description:

This activity supports basic research to understand mechanisms of 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 novel or 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; chemicals and 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 chemical imaging, including ultrafast and synchrotron-based spectroscopies and neutron-based techniques, present unique opportunities for the acquisition of new knowledge in catalysis. This core 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. Multidisciplinary approaches are encouraged by means of multi-PI grants. 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 – Condensed Phase and Interfacial Molecular Science activities have complementary goals in the areas of interfacial science, surface chemistry, and quantum mechanical theory, molecular modeling, and simulation of catalytic-related phenomena. The Catalysis and Solar 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 common issues and in some instances co-support synthetic research for zeolitic, membrane, 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), and the 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), have thrust areas that address catalysis research, and the Center for Nanoscale Materials (CNM) has topics and personnel in 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, homogeneous and bio catalysis, and the surface science and materials aspects of catalysis are funded by separate programs within the Math and Physical Sciences and the Engineering Directorates. 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:

Researchers supported by this CRA have achieved fundamental breakthroughs in catalysis over the last two decades. For instance, significant contributions were made to the molecular-level understanding of catalytic cracking of hydrocarbons in zeolites, reforming of hydrocarbons over supported bimetallic alloys, and desulfurization 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, dramatically improving 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 two decades, one of the most significant accomplishments in homogeneous catalysis was the development of practical catalysts for the metathesis of unsaturated compounds, a reaction that is ubiquitous in organic synthesis and was highlighted by a recent Nobel Prize. Other very significant accomplishments were the discovery of single-site metallocene catalysts for polymerization of alkenes, with one of its major contributors receiving a National Medal of Science, and the development of methods to study the surface science of catalysis, with its major contributor receiving another National Medal of Science. More recently, the low-temperature N_2 activation (the crucial step in ammonia synthesis) was achieved homogeneously. For their achievements, researchers in this program have been widely honored by scientific societies, as they have received most of the awards in Organometallic Chemistry given by the American Chemical Society, most of the fundamental catalysis awards given to U.S. academics by the North American Catalysis Society, two National Medal of Science awards, and the 2005 Nobel Prize in Chemistry.

Mission Relevance:

Catalytic transformations impact virtually all of the DOE energy missions. Catalysts are needed for all or many of the processes to convert crude oil, natural gas, coal and biomass 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 convert environmental pollutants, such as unwanted products of combustion or chemical manufacturing, or replace carcinogenic refrigerants such as chlorofluorocarbons.

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 long-term stability. 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. A special focus is the identification of new carbon-neutral pathways for the catalytic conversion of biologically-derived feedstocks. Those challenges can be met by coordinating fundamental research on chemical synthesis, structural characterization, mechanistic and kinetics studies, and theory-modeling and simulation.

The current challenge in inorganic synthesis is the molecular control of structure, shape, and functionality, by means of rationally designed modular ligands. For biomimetic catalyst development, priority is given to highly versatile ligands and air- or water-resistant complexes. The control of macromolecular structure is a continuing challenge. Priority is given to the design of shape-selective reaction environments.

In solid state synthesis, the current frontier is to produce catalytic materials with nanoscale control of composition, homogeneity, shape, and structure. In particular, emphasis is placed on hybrid organometallic-inorganic porous materials able to catalyze the conversion of multifunctional molecules with high selectivity. Molecular precursors may be converted into solid-state structures with designed chemical functionalities that are durable under reaction conditions. Traditional routes of surface chemistry, aqueous-solution chemistry, and high-temperature chemistry are complemented by softer routes, such as surface-functionalization of nanoparticles with coordination compounds. Organic or biological strategies may then be used to arrange the particles into preconceived patterns possessing unique molecular recognition properties (for example, size, shape, chirality, and hydrophobicity). The interfacial interactions with anchoring ligands, supports, and solvent spheres generate fundamental challenges for exacting characterization but also ways of tuning the reactivity and stability of catalytic materials.

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 discriminated from those that are mere spectators. This is a particularly crucial need in solid-mediated catalysis and biocatalysis.

The study of reaction mechanisms is promoted by the synergistic use of theory, simulation, and experimentation. In particular, identification and structural characterization of the reaction intermediates 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 these reactions present the highest demands on catalysts. While high selectivity has been obtained with homogeneous catalysts in selected instances, heterogeneous or hybrid catalysts require substantially more study, possibly with help from biomimetics and the use of cascade or tandem reactions.

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, one of the challenges is to carry out these selective reactions under solvent-less conditions or in supercritical media or ionic liquids, while maintaining stability. For heterogeneous catalysis, the challenge is to work at extremely high temperature with high selectivity, or extremely low temperature with high activity. New challenges for all types of catalysts have arisen in activating molecules and materials derived from biorenewable resources.

Besides hydrocarbon and carbohydrate chemistry, other challenges reside in the elucidation of the catalytic mechanisms for the synthesis of macromolecular and nano materials. In one example, the catalytic synthesis of carbon or inorganic nanotubes, chirality control has remained elusive because of lack of understanding of the structure-determining steps. In another example, the nucleation and subsequent growth of silicon nanowires from silane or its derivatives on molten gold nanoparticles proceed remain little understood.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009 Request
39,711	39,711	56,927

Performer	Funding Percentage
DOE Laboratories	46%
Universities	54%

These are 3-year average 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 single-site catalysts, and thorough characterization of catalysts and reactions by means of cooperation among groups with complementary expertise in synthesis, structural characterization, intermediate and transition state characterization, dynamics simulation, and kinetics determination.

The convergence of heterogeneous, homogeneous, and biocatalysis is evolving. Ideas and approaches motivated by biological reaction systems will be used to derive new biomimetic homo- or heterogeneous analogues. Examples are the use of long-range or secondary structure and structural flexibility to affect both selectivity and also activity of inorganic catalysts. The mechanisms and pathways for charge transfer and rearrangements following non-thermal activation, such as electrochemical and photochemical activation, will also be addressed.

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 and supercritical media; (f) low-temperature heterogeneous reactions; (g) non-noble metal catalysis; (h) tandem and single-pot catalysis; (i) conversion of biologically-derived feedstocks; and (g) electrocatalytic and photocatalytic activation.

Research Activity: **Separations and Analysis**

Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact: William S. Millman (william.millman@science.doe.gov; 301-903-5805)
Detailee: Larry Rahn, SNL-CA (larry.rahn@science.doe.gov; 301-903-2508)
Team Lead: John C. Miller
Division Director: Eric A. Rohlfing

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 with Heavy Element Chemistry. The portfolio focused around five main thrust areas: 1) Laser-based techniques, including laser spectroscopy and other quantitative analytical techniques; 2) Nanoscale science approaches to separations and analysis, including transport, synthesis of nanoscale pores and structures for separations, analysis of nanoscale materials, and chemical properties unique to nanoscale materials; 3) Ionization processes in analysis, particularly mass spectrometry, including surface preparation and modification, the interactions of ions and molecules, and the transport and acceleration of ions in the presence of applied fields; 4) Metal-adduct complexes for separations, particularly trans-actinide elements, including synthesis of ligands uniquely capable of interacting with specific elements, supramolecular complexes, micelles, and proteins that display unique separation selectivity; 5) Advancing molecular-scale or chemical imaging, including pushing frontiers in spatial and temporal resolution.

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.

Relationship to Others:

The activity is closely coupled to the Department's stewardship responsibility for actinide and fission product chemistry and to its clean-up mission. It emphasizes the separation 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 Science, Chemical Physics, Materials Chemistry, and Atomic, Molecular, and Optical 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 the Advanced Nuclear Energy Initiative.

Major Accomplishments:

This activity is responsible for such notable contributions as the concept of host-guest complexation, for which Professor Donald Cram (UCLA) 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 the Department of Energy and its predecessor agencies in the science that underlies separation processes. The missions of the Department have evolved, and it must now face the legacy of accumulated wastes from the cold war era and the growing emphasis on alternative energy sources. Knowledge of molecular-level processes is required to characterize and treat the extremely complex mixtures associated with cleanup and to predict the fate of associated contaminants in the environment. In addition, separation 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% of total petroleum consumption). Overall, it is estimated that separations processes account for more than 5% of total national energy consumption. This need is increasingly apparent with incipient technologies for alternative energy sources. Separations are essential to nearly all operations in the processing industries and are necessary for many analytical procedures.

Likewise, the Department 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 separation 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 separation science, improved understanding of the underlying science is required to meet the analytical challenges presented by the legacy of the cold war, alternative energy sources, and the future challenges of the Department as its missions and responsibilities continue to evolve.

Scientific Challenges:

Challenges in separation 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 2007	FY 2008	FY 2009 Request
15,860	15,860	28,338

Performer	Funding Percentage (2007)
DOE Laboratories	54%
Universities	46%

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 students and 25-30 postdocs. In addition, 14 programs at national laboratories support numerous senior staff, and additional students and postdocs. Programs at the laboratories are typically multi-investigator efforts on problems that require extensive collaboration by experienced scientists. These programs act as the focal point for specific research efforts vital to the DOE mission. This BES 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 achieve true chemical imaging, i.e., the ability to selectively image selected chemical moieties at the molecular scale and to do so with temporal resolution that allows one to follow physical and chemical processes.

Research Activity:	**Heavy Element Chemistry**
Division:	Chemical Sciences, Geosciences, and Biosciences
Primary Contact:	Lester R. Morss (lester.morss@science.doe.gov; 301-903-9311)
Detailee:	Norman Edelstein, LBNL (nmedelstein@lbl.gov; 510-486-5624)
Team Leader:	John C. Miller
Division Director:	Eric Rohlfing

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 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 themes are the properties that results from the electron orbitals available to these elements, especially the 5f orbitals.

The program emphasis is the chemistry of technetium, uranium, and transuranic elements, driven by the necessity to characterize and control long-lived radioisotopes produced in power reactors and found at Department of Energy (DOE) legacy waste sites. Knowledge of the chemical bonding of legacy actinide and fission products is necessary to predict the properties of these complex mixtures and to treat them. This activity is coupled to the BES Separations and Analysis activity, to actinide and fission product chemistry research in DOE’s Environmental Remediation Sciences Program, and to nuclear fuel cycle research within DOE's Office of Nuclear Energy. The education of undergraduates, graduate students, and postdoctoral researchers in radiochemistry at national laboratories and universities is an important responsibility of this activity.

Unique Aspects:

This activity represents the only source of funding for basic chemical research in the actinides, fission products, and transactinides in the United States. Its major emphasis is to understand the underlying chemical and physical principles that determine the behavior of these elements. 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 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 (nuclear energy, environmental, stockpile stewardship) generally limit their investigations to the chemical and material properties of specific elements and systems of strategic programmatic interest. This activity also has close ties to the BES separations 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. The early goals were to discover new elements and to determine their chemical and physical properties from microscale and tracer experiments. Processes for the separation of plutonium from uranium and fission products on an industrial scale were then developed. The chemistry of the elements through einsteinium (Es, atomic number 99) has been determined with small but weighable quantities. 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 reactions. Specific electronic transitions determined in this activity have proven useful to develop 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; thus 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 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 was 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 caustic solutions found in or near many waste tanks at DOE sites, this activity has had a renewed emphasis on the molecular speciation of the transuranium elements and fission products. Finally, the analytical chemistry methods developed under this activity have broad application across 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 and is the central focus for this program. The 5f orbitals participate in the band structure of materials that contain the light actinide metals and their alloys. Evidence is accumulating that the 5f orbitals participate significantly in molecular compounds, for example, compounds required for advanced nuclear energy systems. Molecular-level information on the geometry and energetics of bonding can now be obtained 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 surfaces of minerals and colloids in solution. Actinide and fission product samples must be handled in special facilities because of their radioactivity, which limits the types of experiments that can be safely conducted.

Sophisticated quantum mechanical calculations that treat spin-orbit interactions accurately need further development so that they can be used to predict the properties of molecules that contain actinides. Development and validation of 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 such as colloidal particles. Surface complexation models can predict the migration of radioactive species; experimental validation of the theoretical properties of models will be the key to understanding the role of the 5f electrons.

Funding Summary:

Dollars in Thousands

FY 2007	**FY 2008**	**FY 2009 Request**
9,427	9,427	18,789

Performer	**Funding Percentage**
DOE Laboratories	81%
Universities	18%
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.

This activity supports research in heavy element chemistry at universities, encouraging collaborations between university and 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, clusters in liquids, 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 research pursues advances in gas-phase chemistry that explore new reactivity patterns, photophysics and photochemistry of actinide ions in their excited states, and 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 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)
Detailee:	Patrick Dobson, LBNL (patrick.dobson@science.doe.gov; 301-903-0340)
Team Lead:	John C. Miller
Division Director:	Eric Rohlfing

Portfolio Description:

This activity supports basic research in analytical, experimental, and theoretical geochemistry; rock physics; and flow and transport of subsurface fluids. The research seeks to understand how earth properties and processes can be imaged, probed, and understood at higher resolution than available with current technology or approaches. It develops analytical methodologies to probe ever smaller mineral domains to track heterogeneous 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 characterize and predict the geophysical signatures of minerals, rock types, and fluids in the earth. 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 enhance our ability to monitor, measure, and validate ongoing geological processes in the earth. It will underlie our ability to track trajectories and rates of chemical and physical processes in the earth. It expands our knowledge 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 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, Energy Efficiency and Renewable Energy, Environmental Management, and Civilian Radioactive Waste Management through support for DOE national laboratory capabilities used by all of these offices. This research activity seeks to provide 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 eighty university research projects.

Relationship to Other Programs:

The Geosciences Program provides approximately 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. BES research activities focus primarily upon the physical and chemical properties of geo-systems with a cognizance of critical biological interactions. This contrasts with BER research programs which primarily focus on biological interactions with the physical and chemical properties of geo-systems, and on DOE site-specific issues.

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. The Geosciences activity also supports BESSRC at the Advanced Photon Source (APS) and X26a at the National Synchrotron Light Source (NSLS). Geosciences research projects, unique BES supported laboratory facilities, and BES funded workshops on Basic Research Needs for Geosciences and in topical areas are the foundations for identifying research opportunities for research and development integration activities between the Office of Science and the applied program offices. Recent Geosciences workshops have produced broadly applicable publications on geosciences user facilities, reactive fluid flow and transport modeling, and geophysical processes and properties that can be imaged for environmental applications. These documents promote BES activities to the science community in areas of importance for the DOE and publicize DOE research interests to the broader science community. The Geosciences Program has led the development of a 512-node super-cluster for Earth Sciences computing at Lawrence Berkeley National Laboratory to link geochemical and geophysical computing applications. The cluster ranked 354^{th} in the world in speed when commissioned a year ago for less than $1M. Geosciences investigators led a National Academy of Sciences study of grand challenges for the earth sciences which was published in March 2008 as "Origin and Evolution of Earth: Research Questions for a Changing Planet." Investigators sponsored by this activity 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, Isotopic Geochemistry, and Molecular Geomicrobiology, and have published a number of recent textbooks.

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 them. Examples of these applications include (but are not limited to): the potential of geophysical imaging of permeability; reactive fluid flow studies to understand contaminant transport and remediation, and geothermal energy production; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict geological 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 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. 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.   New investigations are needed at the smallest scales to study electronic properties, geochemical reactivity, solute properties, and isotopic distributions in both inorganic and organic systems. Facilities such as the Linac Coherent Light Source (LCLS) will provide unique capabilities for Geosciences investigators to probe natural reactivity processes at ultrafast times to provide a new paradigm for understanding geological reaction rates. Mineral-fluid-biological 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 surface-particle-fluid interactions is the 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. 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, electromagnetic, geomechanical, and hydrologic modeling techniques and provide unique support to experimental analysis.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009 Request
21,392	21,392	28,918

Performer	Funding Percentage
DOE Laboratories	52 %
Universities	47 %
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:

In the near term, geosciences research continues its basic activity in fundamental rock physics, fluid flow, and analytical, 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 and how they contribute to mineral-fluid interactions. 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 designing other facilities such as the National Synchrotron Light Source II (NSLS II). They will expand research efforts in nanogeosciences to understand the role of nanophases in geological systems and efforts on understanding the geophysical and geochemical challenges of predicting the fate and transport of CO_2 as sequestration in deep geological formations is tested as a technology option to mitigate greenhouse gas emissions.

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.