## Research Activity: Geosciences Research

Division: Chemical Sciences, Geosciences and Biosciences
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## 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.