Research Activity: Chemical Energy and Chemical Engineering

Division: Chemical Sciences, Geosciences, and Biosciences
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Portfolio Description:

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

Unique Aspects:

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

Relationship to Others:

Coordination of fundamental and applied research efforts in electrochemistry across the government is accomplished by participation in the Interagency Power Working Group where the program manager is the vice chair of The Chemical Working Group. Close coordination with the Battery and Fuel Cell programs in EE-Office of Transportation Technologies is accomplished through joint program meetings, workshops, and strategy sessions. Coordination in the Chemical Engineering area is primarily with the Chemical Industry Team in the Office of Industrial Technologies in EE through participation in the Chemical Industry Vision 2020 planning activity and the development of joint SBIR topics. A similar relationship with the Fuels program in FE has led to joint SBIR topic development. Additional interaction with the Chemical and Transport Systems division in the Engineering Directorate at NSF is accomplished through direct contact.

Significant Accomplishments:

Lithium and lithium ion batteries: The most significant accomplishment in electrochemistry research that was supported by the office was a spin off from early research on the electrochemistry of reactive metals in polar aprotic solvents by the late Charles Tobias of LBNL. It is widely acknowledged that this research (circa 1964) led to the first lithium battery. The same electrolyte solvent systems are still used today in the current generation of rechargeable lithium and lithium ion batteries. Replacements for Chlorofluorocarbons (CFC's): Research in thermophysical properties led to the development of an equation of state used in identifying replacements for CFC's that were responsible for destroying the ozone in the stratosphere**.** Hydrogen bonding in water: Research in molecular simulation led to clearing up controversial neutron scattering results on the nature of hydrogen bonding in water under supercritical conditions. Thin film rechargeable lithium batteries: Research in solid state electrolytes led to a new generation of thin film rechargeable lithium batteries that are about the thickness of saran wrap. Room temperature molten salt electrolytes: Research in molten salt electrolytes led to new room temperature systems that are showing promise in reactive metal systems such as sodium and lithium. The structural origin of water's anomalous properties: A new formalism for the quantification of structural order in water, based on the introduction of two order parameters has been developed.

Mission Relevance:

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

Scientific Challenges:

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

Funding Summary:

Dollars in Thousands

FY 2003	FY 2004	FY 2005 Request
9,779	10,637	10,687

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

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

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

Projected Evolution:

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