Separations and Analysis

Portfolio Description

This activity supports fundamental research to enable predictive understanding, at molecular and nanoscale dimensions, of the basic principles involved in chemical recognition, separation, and analysis. A range of multidisciplinary experimental and computational approaches is employed, inspired by the potential for discovery of new concepts in a broad spectrum of current mission-relevant separation and analysis applications. Separation approaches include those using membranes, adsorption/desorption, complexation, extraction under both standard and supercritical conditions, chromatography and photodissociation. Chemical analysis research goals include improved sensitivity and applicability of ambient imaging mass spectrometry, and new approaches to analysis in complex, heterogeneous environments. Special emphasis is focused on techniques that combine chemical selectivity, spatial resolution and temporal resolution to achieve chemical imaging at the molecular- and nanoscale. Capital equipment funding is provided to enable measurement of separation/recognition properties, and components such as lasers, advanced mass spectrometers, nanoprobes, and microscopes for chemical imaging research.

Unique Aspects

This activity represents the Nation's most significant long-term investment in solvent extraction, ion exchange, and mass spectrometry. The combined activity with Heavy Element Chemistry is the nation's most significant long-term investment in the fundamental science underpinning actinide separations. 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 Other Programs

- The separations-related activity coordinates closely with the Heavy Element Chemistry Program to support the Department's stewardship responsibility for actinide and fission product chemistry and to its clean-up mission.
- Similarly, elements of the Separations and Analysis portfolio benefit from cooperation with the BES Computational and Theoretical Chemistry, Catalysis Science, Condensed-Phase and Interfacial Molecular Science, Geosciences and Materials Chemistry Programs. The analysis research, in particular, is coordinated with a broad range of BES programs benefiting from advanced chemical imaging.
- A number of BES Energy Frontier Research Centers support investigators and topics of relevance to this activity.
- Other federal agencies support investigators and topics that are mutually complementary. Participation in program management working groups assures coordination across the DOE in related areas such as fuel cells and carbon capture/sequestration.

Significant Accomplishments

This activity is responsible for such notable contributions as the concept of host-guest complexation, which was recognized with 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 upon fundamental research on ligand design; the 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.

More recent accomplishments include:

- A new calixerene ligand-based separations process that complexes Cs+ based on research and development work performed by BES researchers at Oak Ridge National Laboratory is being used to clean up waste tanks at Savannah River National Laboratory.
- Significant contributions to the discovery of metal-organic framework (MOF) materials for carbon capture and other gas separations.
- New approaches to ion separations have resulted in related applications (e.g. patents applicable to desalination).
- A revolution in ambient and imaging mass spectrometry is having very broad impacts in the analysis community.
- New approaches for aerosol and particulate analysis that are impacting the atmospheric and climate change research communities.

Mission Relevance
Early relevance to the Manhattan Project and nuclear defense has broadened to cleanup of accumulated legacy wastes from the cold war era, improved efficacy and energy efficiency in industrial chemical and energy production, the growing emphasis on alternative energy sources and climate change, and on the separations and analysis requirements of the nanoscale revolution.

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, adsorption/desorption, crystallization, dispersion, coalescence, and transport properties of new membrane concepts and materials. The development of fundamental principles to guide design and synthesis of ligands, adsorbents, and self-assembled complexants and membranes are also required. These, in turn, pose challenges to analysts to characterize these and related amorphous materials through analysis of scattering data or other methods. Other analytical challenges include direct observation of molecular scale interactions, self-assembly and chemical 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.

Projected Evolution
Separations research will continue to advance the understanding and control of the atomic and molecular interactions between target species and separations media, and the resulting molecular structures, dynamics, kinetics and transport properties resulting in desired meso- and macroscopic functionalities. Particular current interests include such topics as supramolecular recognition; synthesis of new porous materials; interfacial properties at the nanoscale; ligand

design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; solvation in fluids and their interfaces; and drop formation. This fundamental research is motivated by a desire to advance discovery and predictive design of future chemical separations-related concepts enabling efficient and multifunctional capabilities for a broad range of processes. Examples include membrane processes (e.g. separation, reactive separation, and fuel cell membranes), complexation, extraction under both standard and supercritical conditions, ionic liquids, selective adsorption and efficient release using materials such as MOFs, and limited fundamental aspects of chromatography.

Analytical research will pursue the elucidation of ionization, chemical interactions, and excitation mechanisms for optical and mass spectrometry that enable temporal and chemical observation and characterization at the nano- and molecular-scale of systems relevant to DOE's energy interests. One focal point of this research is the underlying science needed to achieve true chemical imaging, i.e., the ability to selectively image desired chemical moieties at the molecular scale with temporal resolution that elucidates physical and chemical processes relevant to energy science.

Additional evolution of the program is anticipated from the growing DOE mission emphasis on alternative energy sources, climate change, and on exploiting the nanoscale revolution for scientific discovery and mission applications. Based on programmatic priorities, this activity does not support areas directly overlapping those supported by complementary programs in DOE or other agencies or any engineering scale up or development of narrowly defined processes, devices or sensors, or research that is directed toward medical applications.