Separation Science

Portfolio Description

(The emphasis of this program is on separation science, not chemical analysis.)

Thematically, fundamental research funded in this program involves studies of *Chemistry at Complex Interfaces*, *Charge Transport and Reactivity*, *Reaction Pathways in Diverse Environments*, *Chemistry in Aqueous Environments*, and *Ultrafast Chemistry*. More specifically, this program supports fundamental research to predict and control the atomic and molecular interactions and energy exchanges determining the efficiency of chemical separations. This basic research is motivated by a desire to advance discovery and predictive design of future chemical separations utilizing novel, multifunctional, and/or energy- and atom-efficient methods; as well as the development and investigation of novel structures with the desired nano-, meso-, and macroscopic functionalities and dynamic and transport properties.

Separations are essential to nearly all operations in processing industries, and fundamental separation science research is particularly critical to address contemporary issues of fuel, feedstock, and effluent processing in all phases of matter. Of special relevance to the Department of Energy, separation science research that is responsive to the report on Basic Research Needs for Environmental Management[1], and in particular, speciation and reactivity of non-equilibrium separation systems, is well-aligned with the goals of this program. Also well aligned are separation science topics addressing the Basic Research Needs reports on Energy and Water[2] and Future Nuclear Energy[3]. However, research focused on understanding the chemical and physical properties of actinide and transactinide elements is better covered under the BES Heavy Element Chemistry Program.

The Separation Science activity does not support applied research, engineering or scale up of processes, mineral or materials processing, devices or sensors, microfluidics, or research directed toward medical or analytical applications. The program does not support the synthesis and testing of separations materials as the primary goal, as these activities are covered under other core research areas.

Scientific Challenges

Research topics include, but are not limited to:

- The structural aspects and molecular dynamics of elementary separation steps at complex solid-fluid interfaces utilizing fast and ultrafast spectroscopy; the influence of nanoscale environments, such as ligands, electrolytes, confining structures, hybrid membranes, solvation or ionic spheres, etc., on separation kinetics and mechanisms at the molecular level;
- The role of amorphous, disordered, and non-equilibrium heterogeneous structures in separation mechanisms and efficiency;
- Ultra-selective separations in diverse aqueous environments (acid/base, saline, high T);
- Reactive and non-reactive separations involving charge transport, complex mixtures and complex interfaces, and non-traditional solvents such as ionic liquids and deep eutectic solvents;
- The influence of electromagnetic or other fields affecting transport and bonding of charged or neutral species; and
- The mechanisms of energy absorption and dissipation in separating systems.

A range of multidisciplinary experimental, theoretical and computational basic research approaches are employed, inspired by the multidimensional and time-dependent complexity of chemical separation problems. In particular, significant challenges are posed by elucidation of principles and novel theoretical and computational approaches underlying complex fluids and aqueous interfaces, and, in general, molecular recognition, interfacial, ionic and weak interactions. Understanding separation phenomena at the atomic and molecular level is pursued to extend that understanding to the nanoscale, mesoscale, and macroscale phenomena to ultimately predict the thermodynamics, kinetics, and dynamics of separations processes.

Projected Evolution

Separations research will continue to advance the understanding and control of the atomic and molecular interactions between target species and separation media, and the resulting molecular structures, dynamics, kinetics, and transport properties resulting in desired meso- and macroscopic functionalities. Recent topics of interest have included 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, and solvation in fluids and their interfaces. This fundamental research is motivated by a desire to advance discovery and predictive design of future chemical separations concepts enabling efficient and multifunctional capabilities for a broad range of processes. Examples include membrane processes, complexation, extraction under both standard and supercritical conditions, ionic liquids, and selective adsorption and efficient release. This program actively pursues better characterization and modeling of the interactions of target ions at liquid-solid and liquid-liquid interfaces to improve separations processes that are broadly applicable to energy and chemical technologies.

Additional evolution of the program is anticipated from the growing emphasis on advanced energy sources, environmental management, 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, including:

- Any engineering scale-up or development of narrowly defined processes, devices, or sensors;
- Microfluidics;
- Research that is directed toward medical applications;
- Research on the transport of subsurface contaminants; or
- The form and mobility of contaminants including wasteforms.

Significant Accomplishments

This activity is responsible for such notable contributions as the concept of host-guest complexations and, more recently:

- A new calixarene 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 materials for carbon capture and other gas separations.
- Simple molecular frameworks with strategically-placed ion binding sites are providing highly efficient and cost-effective reagents for corralling and separating targeted ions such as sulfate from nuclear waste.

- The concept of ion-gated selective gas separations was demonstrated by molecular dynamics simulations, potentially providing for flexible and dynamic control of pore size for both high-permeance and high-selectivity ultrathin membranes for gas separation.
- New membrane-free approaches to ion separations using light rather than electrical energy are impacting related large-scale applications such as desalination.
- Fundamental studies that are following the movement of single dye molecules diffusing through surfactant-filled silica mesopores are providing a detailed, nanoscale view of molecular diffusion pathways in this important class of separations materials.
- A novel process for both the solution-phase capture and direct conversion of carbon dioxide to highly useful methanol has been developed. Fundamental mechanisms for this multi-functional process are now being explored.

Unique Aspects

The research supported by this activity is characterized by a unique emphasis on underlying chemical and physical principles, as opposed to the development of methods, materials, and processes for specific applications. Considering the ubiquity of separations as essential for the sustainable production of fuels and chemicals, and for a large number of pollution prevention and environmental clean-up processes, the outcome from the fundamental separation science research carried out in this program will have significant impact on the energy intensity of these often inefficient processes.

Mission Relevance

Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies, and to support DOE missions in energy, environment, and national security. The Separation Science program is an important component of this effort, particularly to the DOE missions in energy and environment. Nuclear defense work left a substantial amount of legacy waste, and this program pursues fundamental research that underpins technologies to enable eventual permanent disposition. Improved efficacy and energy efficiency in industrial chemical and energy production, as well as the growing emphasis on alternative energy sources make the Separation Science program directly relevant to the DOE's energy mission.

Relationship to Other Programs

- The Separation Science activity coordinates with the BES Heavy Element Chemistry program, which supports research focused on understanding the fundamental chemistry of actinide and transactinide elements.
- This activity maintains a distinct portfolio from other BES activities, such as the Computational and Theoretical Chemistry, Catalysis Science, Condensed-Phase and Interfacial Molecular Science (CPIMS), Geosciences, and Materials Chemistry Programs.
- A number of BES Energy Innovation Hubs and Energy Frontier Research Centers support investigators and topics of relevance to this activity.
- The Separation Science activity produces research outcomes of relevance to programs of the DOE's Office of Energy Efficiency and Renewable Energy and Office of Fossil Energy. Participation in program management working groups assures coordination across the DOE in related areas such as chemical and energy processes.

- Other federal agencies, including the National Science Foundation (NSF), National Institutes of Health (NIH), Environmental Protection Agency (EPA), and the Defense Department, support investigators and topics that are mutually complementary.

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1 https://science.energy.gov/~/media/bes/pdf/reports/2016/BRNEM_rpt.pdf

2 https://science.energy.gov/~/media/bes/pdf/brochures/2017/Energy_and_Water_Brochure.pdf

3 https://science.energy.gov/~/media/bes/pdf/brochures/2017/Future_Nuclear_Energy_Brochure.pdf