

## Separation Science

### Portfolio Description

The Department of Energy (DOE) is concerned with controlling the efficiency of energy and mass flows within systems that utilize the nation's energy-relevant resources including petroleum, natural gas, biomass, minerals, critical materials, air and water. Today, these resources include an abundant supply of atmospheric carbon species as well as plentiful supplies of unconventional feedstocks that contain valuable materials but may otherwise be considered waste. Research in chemical separations is particularly critical for ensuring a sustainable chemical and refining enterprise, enabling sound nuclear waste cleanup and storage strategies, securing essential elements needed for advanced energy technologies, and addressing contemporary issues of fuel, feedstock, and effluent processing in all phases of matter.

The Basic Energy Sciences (BES) Separation Science program funds hypothesis-driven experimental and computational research to discover, understand, predict, and control de-mixing transitions and associated enabling separations technologies. This includes understanding molecular interactions and energy exchanges that determine the efficiency of chemical separations. This program also aims to advance the discovery and predictive design of chemical separation paradigms that may become the basis for solutions to the world's energy challenges. Equipped with an enhanced understanding of the governing principles for de-mixing transitions that take a chemical system from one thermodynamic state to another, it will be possible to gain more precise control of energy and matter transformations of complex domestic resources.

### Scientific Challenges and Opportunities

The Separation Science Program supports emerging fundamental scientific areas within energy-relevant separation science that are in a nascent stage. Additionally, separation science topics that are of interest the Program are outlined in the National Academies of Science, Engineering, and Medicine (NASEM) report *A Research Agenda for Transforming Separation Science* (<https://www.nap.edu/catalog/25421/a-research-agenda-for-transforming-separation-science>).

Select fundamental topics of interest include:

- elucidating factors that cause a separation system to approach mass transfer limitation in the source phase while maintaining selectivity
- enabling and enhancing strategies for critical materials recovery from natural and unconventional feedstocks; for water and environmental management of heavy elements and nuclear waste; and for carbon removal from low-concentration sources
- understanding non-thermal mechanisms that have the potential to drive efficient and selective energy-relevant separations, such as electromagnetic, magneto-reactive, and other means to affect transport and bonding selectively
- discovering and advancing strategies for removal of dilute constituents from a mixture, including but not limited to reactive separation approaches
- generating specific and long-range interactions among trace constituents with the aim of promoting nucleation of a new phase that is enriched in the target species
- discovering novel approaches for dehydration of heterogeneous systems without the application of heat
- designing separation systems that have high selectivity, capacity, and throughput
- understanding temporal changes that occur in separation systems

The above topics are agnostic to the separation system and may include, for example, membranes, framework materials (e.g., metal-organic framework materials), zeolites, ionic liquids, and molecular complexes. Issues of selectivity, capacity, throughput, durability, and energy input are important for most separations, and should be of concern in separation science research, although they may not be the singular focus.

### **Projected Evolution**

Chemical separations are critical to meeting a vast range of societal needs, providing essential products and services that support the nation's activities and supporting an advanced world. Separations research will continue to develop the understanding and control of the atomic and molecular interactions between target species and separation media, and the relevant molecular structures, dynamics, kinetics, and transport properties that govern separations. In addition to the challenges and opportunities listed above, recent topics of interest have included advanced simulations and data science methods to advance separation science. The supported fundamental research is motivated by a desire to advance predictive design of future chemical separations concepts enabling efficient and multifunctional capabilities for a broad range of processes. This program actively pursues better characterization and modeling of the interactions of target species at liquid-solid and liquid-liquid interfaces to improve separations processes that are broadly applicable to energy and chemical technologies.

Based on programmatic priorities, this activity *does not* support the following areas:

- engineering design or scale-up
- development of narrowly defined processes or devices
- desalination
- microfluidics
- sensors
- research directed toward medical or pharmaceutical applications

### **Significant Accomplishments**

Activities within this program are responsible for such notable contributions as pioneering work in the concept of host-guest complexations for chemical separations and, more recently:

- development of novel metal-ion sorbents for improved extraction of actinides and selected fission products, with uses that span nuclear waste cleanup to the production of highly pure yttrium-90 required for radiation therapy treatment of certain cancers;
- development of a novel process for both the solution-phase capture and direct conversion of carbon dioxide to convert a greenhouse gas to highly useful chemicals;
- advancements of methods to follow the movement of single molecules diffusing through mesoporous and nanoporous separations media to provide a detailed view of molecular diffusion pathways in important classes of separations materials;
- significant contributions to the discovery of crystalline metal-organic framework materials with tunable structures for carbon capture and other gas separations.

### **Unique Aspects**

Considering the ubiquity of chemical separations 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. 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 separations or applications. This program is particularly interested in supporting team-based approaches that combine, for example, the expertise of synergist experimental and simulation scientists to address hypothesis-driven separations research.

### **Mission Relevance**

The energy footprint of chemical separations in the business-as-usual world is significant. For example, approximately 5% of in-plant industrial energy use in the United States is attributable to chemical separations, which are embedded in nearly all operations within the processing industries. Some estimates suggest there is a potential 85% reduction in in-plant energy use for separations by improving already deployed separation technologies. This is the scale of the opportunity for particular sectors of the business-as-usual world. The potential impact is greater for technologies that have not yet been deployed. In potential future world scenarios, the domestic energy footprint of chemical separations is significantly larger – for example, consider an increase in the domestic manufacturing sector or a net-zero carbon future. 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 due to the ubiquity of chemical separations in many energy-relevant processes, particularly to the DOE missions in energy and environment. 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 program coordinates with other BES Programs, including Catalysis, Heavy Elements Chemistry, Geosciences, and Materials Science & Engineering.
- The Separation Science program has been involved in recent BES funding opportunity announcements Direct Air Capture as well as Materials and Chemical Sciences Research on Critical Materials.
- Activities in the Separation Science program can form a basis for new research in a number of relevant BES Energy Innovation Hubs and Energy Frontier Research Centers.
- Research outcomes from the Separation Science program are relevant to DOE applied offices such as the Office of Energy Efficiency and Renewable Energy, the Office of Fossil Energy, and the Advanced Research Projects Agency - Energy. Participation in program management working groups assures coordination across the DOE in related areas that span multiple programs.