Materials Chemistry

Portfolio Description

This program supports scientific research on materials with a focus on the *chemical synthesis, chemical control, and chemical dynamics* of material composition and structure across the range of length scales from atomic to mesoscopic, with a view to elucidating fundamental aspects of materials' structure-property relationships. Major scientific areas of interest include: fundamental aspects of the chemical assembly of material structures and control of multi-scale material morphology; synthesis and characterization of novel organic, inorganic, polymeric and composite materials; synthesis and characterization of complex fluids including ionic liquids; study and control of surface and interfacial chemistry and morphology; fundamental electrochemistry of materials; the study of the chemical dynamics and transformations of functional materials in operational environments; and the development of new, science-driven laboratory-based analytical tools and techniques for the elucidation of chemical processes in materials, particularly *in situ* or *in operando* in energy-relevant applications.

Unique Aspects

Research supported in this program advances knowledge in the materials sciences that underpins many energy-related technologies such as batteries and fuel cells; catalysis; energy conversion, transmission and storage; friction and lubrication; high efficiency electronic devices; photonic materials; light-weight, high-strength materials; and materials for advanced separations. The focus on chemistry-based formation and control of new materials and morphologies is complementary to the BES Biomolecular Materials research activity (that emphasizes discovery of materials and systems using concepts and principles of biology) and the Synthesis and Processing Science research activity (that emphasizes physical, rather than chemical, control of structure and properties, and on bulk synthesis, crystal growth, and thin films). The researchers supported by the program benefit from significant use of BES-supported scientific user facilities with their advanced synchrotron x-ray, neutron scattering, electron microscopy and nanoscience tools.

Relationship to Other Programs

The Materials Chemistry research activity is a vital component of the interface between chemistry, materials, physics and engineering. It is necessarily interdisciplinary and cultivates a number of relationships, within BES and DOE, and within the larger federal research enterprise:

- Within BES, this research activity sponsors – jointly with other core research activities, the Energy Frontier Research Center program, and the Joint Center for Energy Storage Research (JCESR), as appropriate – program reviews, Principal Investigators (PI) meetings, and programmatic workshops.
- There are active interactions with the DOE Offices of Energy Efficiency and Renewable Energy (EERE) and Fossil Energy (FE) through workshops, program reviews, PI meetings, and communication of research activities and highlights.
- Within the larger federal research enterprise, program coordination is through the Federal Interagency Chemistry Representatives, which meets annually, and the Interagency Polymer Working Group.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center activities and reviews in the BES Scientific User Facilities Division. BES

further coordinates nanoscience activities with other federal agencies through the National Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology Subcommittee that leads the National Nanotechnology Initiative.

- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the NSTC Subcommittee on the Materials Genome Initiative.
- There are particularly active interactions with the National Science Foundation (NSF) through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.

Significant Accomplishments

The Materials Chemistry research activity has resulted in a variety of scientific accomplishments including the discovery of new superconducting materials, the discovery of the first organic magnet above room temperature, and the demonstration of new analytical techniques for surfaces and interfaces that have had significant impact in their respective fields.
Recent accomplishments include:

- The first demonstration of a metal organic framework material that shows both stable micropores and good charge mobility, relevant to energy storage technologies;
- The discovery of metal-containing polymers capable of white light emission, with significance for the future development of polymer-based solid-state lighting materials;
- A new understanding of the behavior of charged particles in ionic liquids that helps explain the low electrical conductivity of many ionic liquids and is expected to lead to the design of new and improved ionic liquids for energy-relevant applications;
- Demonstration of a method to completely polarize nuclei near optically polarized nitrogen-vacancy centers in diamond at room temperature, which can be applied to enhance the sensitivity of NMR/MRI experiments in bulk materials;
- Discovery and elucidation of the mechanism of dysprosium doping to boost the performance of a known thermoelectric material (TAGS-85) by 15%; and
- Fundamental studies on materials aspects of a micro-transfer printing process led to the development of micro-contact printed solar cells (and their commercialization by Semprius Inc.) that set the world record for high concentration photovoltaic module efficiency (33.9%) in January 2012.

Mission Relevance

The Materials Chemistry program supports research to generate fundamental knowledge based on the principles of chemistry about the creation, manipulation and functional behavior of materials that will underpin the future development of energy-relevant technologies including systems for energy storage, transformation, and utilization, with levels of performance superior to the current state of the art.

Scientific Challenges

The Materials Chemistry research activity seeks to explore and advance the frontier of accessible functional materials, through the application of the methods and principles of chemistry. Doing so requires addressing specific scientific challenges and opportunities, such as those identified in the BES Advisory Committee's reports, including *Directing Matter and Energy: Five Challenges for Science and Imagination* (report link) and *From Quanta to the Continuum:*

Opportunities for Mesoscale Science (report link). Challenges and opportunities identified in these reports include:

- Discovering new methods to design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties, taking advantage of the recent and ongoing development of theoretical methods and tools;
- Characterizing and controlling matter far away from equilibrium;
- Mastering defect mesostructure and its evolution by characterizing and controlling the patterns and evolution of mesoscale heterogeneity;
- Directing assembly of hierarchical functional materials through the integration of disparate materials classes across a range of length scales from molecular to macroscopic.

Each of these challenges and opportunities may potentially be addressed by the application of chemical principles to the design, synthesis and transformation of materials.

Projected Evolution

The overarching goal of materials chemistry research is to provide the *knowledge* needed to design and produce materials with tailored properties from first principles. This program will make progress towards that goal by emphasizing hypothesis-driven research on the chemistry-based synthesis of materials and/or morphologies that have the potential to enable next-generation energy-relevant technologies, and research on the chemical transformations occurring in functional materials in the operating environment. It will include the study of chemical processes that direct and control the covalent and non-covalent assembly of materials, discovery of synthetic methods to tailor the symmetry and dimensionality of crystalline and non-crystalline lattices, and the utilization of chemistry to control interfacial properties and interactions of materials. New approaches to the integration of theory and experiment leading to new materials design ideas and opportunities for predictive materials discovery may also be supported.