Materials Chemistry

Portfolio Description

This research activity supports basic research in chemical synthesis and discovery of new materials. The major programmatic focus is on the discovery, design and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties. Major thrust areas include: nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials and complex fluids; surface and interfacial chemistry including electrochemistry; and the development of new, science-driven laboratory-based analytical tools and techniques.

Unique Aspects

Research supported in this activity underpins many energy-related technological areas such as batteries and fuel cells, catalysis, energy conversion and storage, friction and lubrication, high efficiency electronic devices, hydrogen generation and storage, light-emitting materials, light-weight high-strength materials, and membranes for advanced separations. The focus on exploratory chemical formation of new materials is complementary to the emphasis on bulk synthesis, crystal growth, and thin films in the BES Synthesis and Processing Science activity. It complements the BES Biomolecular Materials Research Activity (whose emphasis is on discovery of materials and systems using concepts and principles of biology) and the Synthesis and Processing Science Research Activity (whose emphasis is on 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 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, within DOE, and within the larger federal research enterprise:

- Within BES, this research activity sponsors, jointly with other core research activities and Energy Frontier Research Centers as appropriate, individual projects, program reviews, contractor meetings, and programmatic workshops.
- Within DOE, program coordination is through the Energy Materials Coordinating Committee with representatives from the Offices of Science , National Nuclear Security Administration, Fossil Energy, Environmental Management, Nuclear Energy Science and Technology, Energy Efficiency and Renewable Energy, and Electricity Delivery and Energy Reliability.
- Within the larger federal research enterprise, program coordination is through the Federal Interagency Chemistry Representatives, which meets annually, and the Interagency Polymer Working Group. There are particularly active interactions with the National Science Foundation, through joint workshops and joint funding of appropriate and select activities (two are currently ongoing).
- 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's Nanoscale Science, Engineering, and Technology

subcommittee, which leads the National Nanotechnology Initiative.

Significant Accomplishments

The Materials Chemistry Research Activity has a long history of accomplishments. Some can already be considered to have had significant impact on science or technology:

- The first organic magnet at any temperature (and later the first organic magnet above room temperature) – these discoveries created a new class of functional materials and a thriving new field of scientific research that in turn is expected to have a huge impact on technologies based on magnetic materials, such as spintronics;
- The first all-organic superconductor and the highest-T_c organic superconductor;
- The development of neutron reflectivity for non-destructive study of surfaces and interfaces with an unprecedented depth resolution of one-half nanometer; and
- The development of combinatorial materials chemistry, a revolutionary technique for materials discovery that has found wide application in science and industry was supported by this activity (e.g., the founding of Symyx).

Others are more recent but already show promise of significant impact:

- Demonstration of extremely large enhancements in thermoelectric efficiency in semiconductor nanowires (a factor of 100 for silicon);
- Advances in the design and fabrication of solution-processable tandem solar cells – inexpensive plastic solar cells with > 10% conversion efficiencies may now be within reach;
- The development, using block copolymers, of a self-patterning and self-organizing resist that enables fabrication of electronic components at an areal density of 10 Terabit/in^2 (more than 15 times greater than previously possible); and
- Quantitative determination and theoretical confirmation of the long-elusive nanometer-scale structure of Nafion®, the current gold-standard for fuel cell membrane material.

Mission Relevance

Materials are the tool box that enables the development of the next generation of energy technologies. The mission of this program is to build and extend that tool box by utilizing chemistry and “chemical thinking” to control the assembly, structure and function of materials and materials constructs at unprecedented levels. The resulting science and new materials have potential for long-term benefit to energy-relevant technologies, including: batteries and fuel cells, electro-catalysis, energy conversion and storage, friction and lubrication, high-efficiency electronic devices, light-emitting materials, light-weight high-strength materials, membranes for advanced separations, solar energy conversion and materials for carbon capture.

Scientific Challenges

The Materials Chemistry Research Activity seeks to explore and push back the boundary that divides those functional materials which are now possible to design and synthesize from those which are not. Doing so requires tackling a number of scientific challenges, including a cross-cut of the overarching Grand Challenges identified in Basic Energy Sciences Advisory Committee’s (BESAC) *Directing Matter and Energy* report. Two especially important challenges are:

- *building an understanding (experimentally, conceptually and computationally) of materials phenomena which could enable atom-by-atom design and synthesis of innovative materials;*

- *the development and use of powerful new theory/modeling and physical/chemical characterization tools that can accelerate materials discovery*.

In addition, a number of particular energy-science challenges, identified in the BES Basic Research Needs workshops and reports, are conducive to materials chemistry approaches. These include those involving materials with tailored properties as well as those whose design and syntheses are amenable to chemical thinking: Electrical Energy Storage (including battery science, electrolyte phenomena, storage of ions in high porosity materials, and new probes of energy-storage chemistry); Catalysis for Energy, Solar Energy Utilization; Solid-State Lighting; Carbon Capture and Storage; and Superconductivity.

Projected Evolution

With the completion of the recent cycle of BES Basic Research Needs (and other) workshops and reports, the scientific community has articulated very clearly those areas of science and materials which are most relevant to energy. All of the reports variously identify the overarching goal of materials chemistry research as providing the knowledge needed to design and produce new materials with tailored properties from first principles. This program will make progress towards that goal by increasing activity in the following areas: (1) Development of new chemical means to direct and control the non-covalent assembly of materials, such as strategies to organize electron donors and acceptors; (2) Creation of ways to tailor the symmetry and dimensionality of crystalline lattices; (3) Utilization of chemistry to control and design interfaces between dissimilar materials. All of these activities will be conducted on materials that have potential for use in the next generation energy technologies, including research to underpin understanding of new approaches and chemistries related to carbon capture. The program will seek to increase the proportion of research in classes that demonstrate promise in providing the properties required for energy solutions. Some examples of these classes include complex inorganic oxides, metamaterials, and liquid crystals with novel electronic, magnetic, photonic and thermal properties.