Materials Chemistry

Portfolio Description

This program supports research on materials with a focus on the role of chemical reactivity, chemical transformation, and chemical dynamics in material composition, structure, function, and lifetime across the range of length scales from atomic to mesoscopic. The overarching goals of materials chemistry research are to elucidate fundamental chemical aspects of materials' composition-structure-property relationships and to provide the knowledge needed to design and produce materials with tailored properties from first principles.

Program emphases are on hypothesis-driven basic research on the chemistry-based synthesis of materials and/or morphologies that have the potential to enable next-generation, energy-relevant technologies, and on the chemical transformations that occur in functional materials in operating environments. Included are the study of chemical processes that direct and control the covalent and non-covalent assembly of materials, the discovery of the mechanistic detail of chemical transformations and dynamics in materials, the utilization of chemistry to control interfacial properties and interactions of materials, and the development of science-driven tools and techniques to achieve fundamental real-time understanding of materials assembly pathways and materials properties. New approaches to materials discovery involving the integration of theory and experiment are supported within the portfolio.

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 (https://science.energy.gov/bes/community-resources/reports/), including *Directing Matter and Energy: Five Challenges for Science and Imagination* and *From Quanta to the Continuum: Opportunities for Mesoscale Science*. 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 continuing to emphasize 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. 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 new classes of organic, inorganic, polymeric, and composite materials (crystalline and non-crystalline) with novel functionality; control of surface and interfacial chemistry and morphology; fundamental electrochemistry of solid-state materials; chemical dynamics and transformations of functional materials in operational environments; and 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.

Research primarily aimed at the optimization of synthetic methods or of properties of materials for applications, and research with a primary goal of device fabrication and testing, will be discouraged.

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:

- Discovery of a new class of materials, a porous polymer/metal organic framework(MOF) hybrid material, termed 'polyMOFs,' that were shown to exhibit effective gas separation properties;
- Developing a synthetic route to ultra-fine jagged Pt nanowires with highly stressed, under-coordinated surface configurations, that exhibit record high mass activity for the oxygen reduction reaction, doubling the previous record;
- Design of nanostructured MoS_2 electrodes having pathways for both fast ion and electron transport that show dominantly capacitive behavior, allowing for fast charging times;
- Creation of a new crystalline porous material with designed pore partitions that exhibits near-record carbon dioxide uptake;
- Demonstration that controlling the nanostructures of the layered dichalcogenides, MoS_2 and WS_2, dramatically enhances their catalytic activity toward the hydrogen evolution reaction;
- 3-D imaging of nanoparticles rotating freely in a liquid with near-atomic resolution that enables understanding of their growth mechanisms in order to advance the development of nanomaterials for energy applications;
- First demonstration of a MOF material that shows both stable micropores and good charge mobility, relevant to energy storage technologies; and
- Discovery of single-crystal nanowires composed of hybrid organic-inorganic lead halide perovskites as the most efficient nanowire lasers known.

Unique Aspects
Research supported in this program advances fundamental knowledge in the materials sciences that underpins many energy-related technologies such as energy harvesting, conversion, transmission, and storage devices; high-efficiency catalysts and electrocatalysts; friction and

lubrication materials; high-efficiency electronic devices; advanced 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 (with an emphasis on discovery of materials and systems using concepts and principles of biology) and the Synthesis and Processing Science research activity (with a focus 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 scientific user facilities with their advanced x-ray, neutron scattering, electron microscopy and nanoscience tools.

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 harvesting, storage, transformation, and utilization, with levels of performance superior to the current state of the art.

Relationship to Other Programs
The fundamental research supported by the Materials Chemistry program serves as an interface between chemistry, materials science, 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 Centers 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 Materials Representatives (FIMaR), the Federal Interagency Chemistry Representatives (FICR), 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 Nanotechnology Coordination Office (NNCO), which provides technical and administrative support to the National Science and Technology Council (NSTC) Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) for the National Nanotechnology Initiative (NNI).
- 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 (MGI).
- 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.