Biomolecular Materials

Portfolio Description

This activity supports fundamental research in the discovery, design, and synthesis of functional and hierarchical materials, including the materials aspects of energy conversion processes based on principles and concepts of biology. Since biology provides a blueprint for translating atomic and nanoscale phenomena into mesoscale materials that display complex yet well-coordinated collective behavior, the major programmatic focus is on the hypothesis-driven creation of energy-relevant versions of these materials optimized for harsher, non-biological environments. New fundamental science approaches are sought that will lead to predictable and scalable synthesis of novel, hierarchically structured polymeric, inorganic, and hybrid functional materials *in vitro* with controllable morphology, content, behavior, and performance.

Major thrust areas include: harnessing or mimicking the energy-efficient synthesis approaches of biology to generate new optimized materials for a broad range of non-biological conditions; bioinspired self-, directed-, and dissipative-assembly approaches with control of mechanisms and kinetics to form materials that display novel, unexpected properties that are far from equilibrium; adaptive, resilient materials with self-repairing capabilities; and development of science-driven tools and techniques to achieve fundamental real-time understanding of synthetic and assembly pathways, and to enable active, precise manipulation of structure and function. Integrated theoretical and experimental approaches to understand how materials complexity leads to new functionalities, development of new design ideas, and opportunities for accelerated discovery are emphasized.

Scientific Challenges

Since biology has already figured out ways in which matter, energy, entropy, and information are organized and/or manipulated across multiple length scales, the challenge for us is to understand, adapt, and improve upon them so that they will become valuable and practical under a broader range of harsher, non-biological conditions. The major scientific challenges that drive the Biomolecular Materials activity directly correspond to the scientific challenges laid out in the report *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* (https://science.energy.gov/bes/community-resources/reports):

- Realizing targeted functionality in materials by mastering spatial and temporal control of the synthesis and assembly of hierarchical architectures and beyond-equilibrium matter, and so build into synthetic materials a new level of information content approaching that of biological materials.
- Development of predictive models, including the incorporation of metastability, to guide the creation of beyond-equilibrium matter, and pursue the opportunity to go even beyond what nature has achieved to advance the frontiers of energy science.
- The development of methods for in situ characterization of spatial and temporal evolution during synthesis and assembly.

Programmatic challenges also directly correspond to four of the five scientific grand challenges in basic energy sciences, as described in the report, *Directing Matter and Energy: Five Challenges for Science and Imagination* (https://science.energy.gov/bes/community-resources/reports):

- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from complex correlations of the atomic and electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?
- How do we characterize and control matter away--especially very far away--from equilibrium?

Additional challenges directly correspond to the objectives laid out in the reports *From Quanta to the Continuum: Opportunities for Mesoscale Science* and *Computational Materials Science and Chemistry* (https://science.energy.gov/bes/community-resources/reports):

- Discovering, controlling, and manipulating complex mesoscale architectures and phenomena to realize new functionality.
- The development and use of powerful new theory/modeling and physical/chemical characterization tools that can accelerate materials discovery.

Projected Evolution

The activity will expand research on methods to create mesoscale materials with high fidelity and in appreciable quantities. For dissipative- and directed-assembly approaches, programmatic focus will be on: spontaneous assembly-disassembly and reconfiguration, the ability to respond *en masse* to directed and environmental cues, coordination of collective response to multiple signals, defect management, ability to self-repair and rebuild structure, and capability for self-replication and autonomous function. This activity will also expand research to design and create next-generation materials for energy conversion and storage with programmable selectivity and transport based on biological gating and pumping functions, and to understand and precisely control bioinspired mechanisms for directing synthesis and function at organic-inorganic interfaces.

Research that does not have a clear focus on materials science or is aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, and biomedical research will be discouraged.

Significant Accomplishments

Although relatively new within BES, the Biomolecular Materials activity has produced accomplishments that show promise of significant impact:

- A process for inserting short, narrow, subnanometer carbon nanotubes (CNTs) that mimic biological ion channels into synthetic lipid membranes. The confined water in the CNTs formed one-dimensional water wires that drastically boosted the proton transport rate to an order of magnitude faster than bulk water and faster than the state-of-the-art membrane in fuel cells.
- A new strategy for modulating entropic and enthalpic attractive interactions between particles that enables crossover between two distinct assembly pathways.
- Synthesis of defect-free, 2-dimensional protein crystals using a simple chemical-bonding and design strategy that display highly desired counterintuitive mechanical behavior—they expand or contract equally in both directions when stretched or compressed. Such

materials absorb vibration; resist shear, indentation, and fracture; may enable active tuning; and are attractive for use in highly resilient, tunable, lightweight packaging and electronics.

- A new self-regulating process for polymer self-healing using a fluid secretion process inspired by wound-healing processes of living systems.
- A new class of 3D porous, crystalline framework materials formed by spherical protein nodes that assemble as designed through directed interactions between these nodes, metal ions, and organic linkers.

Unique Aspects

Basic research supported in this activity underpins DOE's mission to develop future, transformative energy technologies in areas such as energy conversion, transduction, and storage; light-weight/high-strength materials; efficient membranes for highly selective separations; and energy-efficient, low-temperature synthesis of materials. Current scientific thrusts balance grand challenge and use-inspired basic research, and require strong interactions among biology, chemistry, physics, and computational science disciplines. This activity's focus on new energy-related materials by exploiting biological principles and concepts is complementary to the focus on chemistry-based formation and control of new materials and morphologies of the Materials Chemistry research activity, and to the emphasis on physical, rather than chemical, control of structure and properties and on bulk synthesis, crystal growth, and thin films of the Synthesis and Processing Science research activity. The Biomolecular Materials activity's focus on the intersection of biology and materials sciences complements the Physical Biosciences activity in the Chemical Sciences, Geosciences, and Biosciences Division, which focuses on biochemical, chemical and molecular biological approaches to further our understanding of the ways plants and/or non-medical microbes capture, transduce, and store energy.

Mission Relevance

Biology offers an extraordinary source of inspiration for the development of new materials with precise control of collective self-healing, self-regulating, catalytic, and energy-harvesting, -conversion, -transduction, and -storage behavior. Basic research supported by the Biomolecular Materials activity underpins development of a broad range of energy-relevant materials and technologies such as lighter and stronger materials to improve fuel economy, materials to control transport across membranes and make separations and purification processes more efficient, energy-efficient synthesis and assembly of functional materials, and processes that can convert light, carbon dioxide, and water to fuels.

Relationship to Other Programs

The Biomolecular Materials program is a vital interdisciplinary component of the materials sciences that interfaces materials sciences with biology. This interfacing results in active relationships within BES, within 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.