Research Activity: **Biomolecular Materials**

Division: Materials Sciences and Engineering
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Portfolio Description:

This activity supports fundamental research in the design and synthesis of novel materials and material assemblies by using concepts and principles of biology. The major programmatic emphasis is on exploring molecules and processes of the biological world that could be utilized or mimicked in designing novel materials, processes, and devices with potential energy significance in support of DOE's mission. Major thrust areas include:
(1) understanding, controlling, and building complex structures by self-, directed- and hierarchical assembly, the approach widely found in Nature; (2) biomimetic and/or bioinspired routes to synthesize energy relevant materials, e.g., semiconductor, ferroelectric, optical, and magnetic materials; (3) design and synthesis of functional materials and complex structures with properties and capabilities found in Nature, e.g., emergent behavior, self-repair;
(4) design and synthesis of multi-component, e.g., inorganic, organic, polymeric and biological, materials that will develop new functions and collective properties that are not achievable in individual components alone;
(5) materials aspects of biological energy conversion and storage; and (6) development of science-driven "Tools and Techniques" for the characterization of biomolecular and soft materials.

Unique Aspects:

Basic research supported in this activity underpins many energy-related technological areas such as energy conversion and storage, light-weight and high-strength materials, efficient membranes for highly selective separations, and advanced catalytic systems/architectures similar to natural enzymes with high specificities and high turnover ratios. Focus of this activity on the exploitation of biology in the quest for new materials is complementary to the emphasis on: (1) exploratory chemical synthesis of materials and chemical control of properties in the Materials Chemistry activity; and (2) physical principles and concepts such as nucleation, diffusion, solidification, and phase transformations in the Synthesis and Processing Science activity. Similarly, the Biomolecular Materials activity, with its principal interests in areas at the intersection of biology and materials sciences, complements the Energy Biosciences activity in the Chemical Sciences, Geosciences and Biosciences Division, whose focus is on areas where biological sciences intersect with energy-relevant chemical sciences. Significant interactions and collaborations exist between the principal investigators in this activity and other core research activities, e.g., with the X-Ray and Neutron Scattering activity for the characterization of new materials by use of advanced scattering/spectroscopic tools at BES supported synchrotron and neutron facilities. Many of the scientists performing work at the bio/nano interface sponsored by this activity are also leaders of corresponding science thrust areas at the BES Nanoscale Science Research Centers supported by the Scientific User Facilities Division.

To a large measure, the scientific thrusts pursued in this portfolio are multi-investigator and multi-disciplinary type as they require strong interactions between the physical sciences and life sciences. Investigators supported in this program are world leaders in biomolecular materials, encompassing topics such as self- and directed assembly, interfacial science, bio-nanoscience, hybrid (organic-inorganic-biological) materials, phospholipid membrane biophysics, and bioinspired materials and concepts in friction, adhesion, and lubrication. Several investigators in this program are pioneers of novel synthetic strategies such as the use of biomolecules as catalysts and/or templates for materials synthesis, combinatorial chemistry for new materials discovery, generation of a bacterium with unnatural amino acid genetic code, bio-inspired polymer architectures that self-assemble into pre-designed macroscopic structures, DNA-directed assembly of nanocrystals, and development of novel tools and techniques to probe biomolecular materials and processes. The activity has sought to maintain an optimal balance between "discovery-class research" and "use-inspired basic research," and will continue to identify and support high-risk, high-impact research that can potentially result in ground-breaking discoveries.

Relationship to Other Programs:

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

- Within DOE, there is coordination through the Energy Materials Coordinating Committee (EMaCC) which involves representatives of the Offices of Science (SC), National Nuclear Security Administration (NNSA), Fossil Energy (FE), Environmental Management (EM), Nuclear Energy Science and Technology (NE), Energy Efficiency and Renewable Energy (EERE), and Electricity Delivery and Energy Reliability (OE).

- Within BES, there are jointly funded programs between the DOE national laboratories and universities (about six currently), joint program reviews, joint contractor meetings (with EERE), and workshops.
- The program coordinates through the NSTC Nanoscale Science, Engineering, and Technology subcommittee (NSET), which formulated the National Nanotechnology Initiative (NNI). The NSET subcommittee coordinates the NNI among a large number of federal agencies.
- Very active interactions with the National Science Foundation (NSF) and National Institutes of Health (NIH) through joint workshops and joint support of National Academy studies in relevant areas (two currently active).

Significant Accomplishments:

This program is responsible for pioneering the combinatorial materials synthesis approach for the discovery of new inorganic materials. Combinatorial chemistry was previously developed for high-throughput synthesis of a library of biologically active molecules to assist in drug discovery. Biosynthetic routes found in Nature (e.g., in marine sponges, magnetotactic bacteria) have been harnessed to produce a wide variety of semiconductor, ferroelectric, and magnetic nanocrystals under mild conditions and under environmentally benign conditions. Another remarkable achievement is the development of a method to genetically encode unnatural amino acids (beyond the common twenty) with diverse physical, chemical, or biological properties in bacteria *E.Coli* and mammalian cells. The expanded amino acid genetic code makes it possible to synthesize proteins incorporating unnatural amino acids, thereby producing “synthetic” analogs of proteins. This can eventually lead to our ability to generate entirely new functional biomolecular materials, and even make it possible to go beyond proteins to prepare the long-sought-after mono-disperse versions of industrial polymers such as polyesters and polyimides. A novel strategy to stabilize liposomes as well as to immobilize them on surfaces has been demonstrated by use of nanoparticles. This strategy addresses the longstanding challenge of enhancing the stability and durability of phospholipid bilayer structures so that they can be used in materials applications as smart materials, nanoscale chemical reactors for massively parallel synthesis, etc. Integrating carbon nanotubes with proteins and living cells has recently been accomplished by use of synthetic polymers appended with sugar molecules, and surprisingly, the hybrid composite (nanotube-polymer-sugar molecule) was found to be non-toxic to cells. Nanotube-living cell hybrid structures combine the biological functions of cells with electronic and optical properties of nanotubes as a model multi-functional, biomolecular material construct. A broad-spectrum light-harvesting system that self-assembles into precisely shaped rods like tobacco mosaic virus and mimics the antenna in photosynthetic bacteria has been developed. Recently, the DNA-guided assembly of nanoparticles into three-dimensional crystalline assemblies has been demonstrated for the first time.

Mission Relevance:

The research supported in this activity addresses many of DOE’s strategic themes including Energy Security, Scientific Discovery and Innovation, and Environmental Responsibility. The research in this portfolio underpins many energy-related technological areas such as catalysis; energy conversion and storage; friction, adhesion, and lubrication; hydrogen generation and storage; light-weight high-strength materials; and membranes for advanced separations.

Scientific Challenges:

The major scientific challenges that drive the Biomolecular Materials activity directly correspond to four out 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.* The four grand challenges are: (1) How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties? (2) How do remarkable properties of matter emerge from complex correlations of the atomic and electronic constituents and how can we control these properties? (3) How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems? And, (4) how do we characterize and control matter--especially very far away--from equilibrium? Since biology has already figured out, albeit over several billion years, ways in which matter, energy, entropy, and information are organized and/or manipulated, the challenges for us is to understand, adapt, and improve upon them so that it will become valuable and practical under a broader range of non-biological and harsher conditions.

Funding Summary*:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
46,439	43,430	61,310

Performers (FY2005)	Funding Percentage**
DOE Laboratories	49%
Universities	51%

*Represents the combined totals for Materials Chemistry and Biomolecular Materials.
**Based on FY2007
These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

This activity will strive to maintain a well-balanced research portfolio that addresses both “discovery-oriented” and “use-inspired” basic science. It will also seek to support high-risk scientific pursuits that are curiosity-driven, and develop new multi-disciplinary approaches, with biology, chemistry, physics, and computational science playing major roles, to model, design, and synthesize novel materials with unique functionalities. The program will continue to seek a fundamental understanding of thermodynamic, kinetic, and dynamical aspects of “self-assembly” to produce both equilibrium and non-equilibrium material structures. In addition to the current thrust areas mentioned above, the program will expand in the following areas: self-healing and self-repairing materials; effective strategies for interfacing biological and non-biological materials systems in search of multi-functional materials and emergent behavior; synthetic enzymes; material architectures for efficiently integrating light-harvesting, photo-redox, and catalytic functions to convert carbon dioxide into liquid fuels; and biomolecular functional devices that take inspiration from biological gates, pores, channels, and motors.