Research Activity: **Materials Chemistry**

Division: Materials Sciences and Engineering

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Portfolio Description:

This activity supports basic research in the design and synthesis of novel materials and material constructs with an emphasis on the chemistry and chemical control of structure and collective properties. Major thrust areas include: (1) nanoscale chemical synthesis and assembly–synthesis of nanoscale materials, manipulation of their properties, and organization of nanoscale materials into macroscopic structures; (2) solid state chemistry–exploratory synthesis and discovery of new classes of electrical conductors and superconductors, magnets, thermoelectric and ferroelectric materials, and porous materials with controlled porosities and tailored reactivities; (3) polymers–exploring and exploiting the self-assembly of block copolymers, polymer composites, and polymers with novel electronic and optical properties; (4) surface and interfacial chemistry–electrochemistry, electro-catalysis, friction, adhesion and lubrication at the nanoscale, and development of new, science-driven, laboratory-based analytical tools and techniques; and (5) biomolecular materials–biomimetic/bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology.

Unique Aspects:

Basic research supported in this activity underpins many energy-related technological areas. Focus of this activity on exploratory chemical synthesis and discovery of new materials is complementary to the emphasis on bulk synthesis, crystal growth, and thin films in the Synthesis and Processing Science activity. Similarly, the Biomolecular Materials activity with a focus on innovative materials complements the Energy Biosciences research, whose focus is on the chemical aspects of biomolecular systems. Significant interactions and collaborations exist between the principal investigators in this activity and 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 nanoscience-related work sponsored by this activity are also leaders of science thrust areas at the BES Nanoscale Science Research Centers.

A sizeable portion of the scientific thrusts pursued in this portfolio are multi-investigator and multi-disciplinary in nature. Investigators supported in this program are world leaders in solid state NMR and MRI, neutron reflectivity of soft matter, organic magnets, organic conductors and superconductors, biomolecular materials, polymer interfaces, nanoscience, organic-inorganic composite materials, basic science of tribology, and advanced inorganic materials including quasicrystals. Several investigators in this program are pioneers of novel instrumentation/ techniques such as high resolution MRI outside the magnet (Pines/Lawrence Berkeley National Laboratory, neutron reflectometers (Felcher/Argonne National Laboratory and Russell/University of Massachusetts), combinatorial materials chemistry for new materials discovery (Schultz/Scripps Research Institute), the surface force apparatus (Israelachvili/UC Santa Barbara and Steve Granick/University of Illinois, Urbana-Champaign), and spin-polarized metastable helium scattering (El-Batanouny/Boston University). The program has sought to identify and support high-risk, high-impact and often ground-breaking research, and will continue to do so.

Relationship to Other Programs:

The Materials Chemistry program is a vital component of the materials sciences that interfaces chemistry, physics, biology, and engineering. This interfacing results in very active relationships.

- Within BES, there are jointly funded programs in the DOE national laboratories and universities (about 10 currently), joint program reviews, joint contractor meetings, and programmatic workshops.
- 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).
- Programs principal investigators are collocated and occasionally co-funded by EERE (batteries and fuel cells, green chemistry, solar energy conversion, and hydrogen storage), FE (catalysis and advanced materials research), and NNSA-Defense Programs (nanoscience research).

- Within the federal agencies, the program coordinates through the Federal Interagency Chemistry Representatives (FICR) which meets annually; the Interagency Power Working Group, which meets annually to coordinate all federal electrochemical technology (e.g., battery and fuel cell R&D) activity; the Interagency Polymer Working Group; and the NanoScience, Engineering, and Technology committee (NSET), which formulated the National Nanotechnology Initiative (NNI) and is currently a sub-committee of the National Science and Technology Council. This last committee meets monthly to coordinate the NNI.
- Very active interactions with the National Science Foundation (NSF) and National Institutes of Health (NIH) through joint workshops and joint funding of select activities as appropriate (two currently active).

Significant Accomplishments:

This program is responsible for pioneering the combinatorial materials chemistry approach for the discovery of new materials (Schultz, 1995). It is also responsible for the discovery of the first organic magnet (Miller and Epstein, 1986), the highest-T_c organic superconductor (Williams et al. 1990), the first all-organic superconductor (Williams et al. 1996), and the first room temperature organic magnet (Miller and Epstein, 1991). The latter discovery created a new field of research, which has grown substantially since then, and has transformed organic magnets from a scientific curiosity to a thriving scientific activity and is expected to have a huge impact on spintronics-based technologies. Recently, the first material that simultaneously exhibits bistability in three physical channels – electronic, magnetic and optical – was discovered (Haddon, 2002). A new approach involving the use of ordered intermetallic materials as fuel cell electrodes has been developed and offers great promise for finding a non-platinum, direct fuel cell that uses organic liquids (e.g., methanol and ethanol) as fuel (DiSalvo and Arbuna, 2003). A biomolecular route found in nature has been harnessed to produce a wide variety of photovoltaic and semiconductor nanocrystals at low temperature and under environmentally benign conditions (Morse, 2003, 2005). A truly remarkable recent achievement is the generation of a bacterium with a 21 amino acid genetic code, which can eventually lead to our ability to generate entirely new functional materials (Schultz, 2003, 2004, 2005). It will also be possible to extend this technology beyond proteins to prepare the long sought after monodisperse versions of industrial polymers such as polyesters and polyimides.

The program also pioneered the development of several cutting-edge techniques for probing materials, e.g., neutron reflectivity for the study of interfaces, buried interfaces, and interfacial phenomena in magnetic materials, polymers, colloids, biomaterials, and other complex, multicomponent materials. Every neutron scattering facility in the world now has neutron reflectometers, which are in great demand. The program pioneered and developed the use of laser polarized xenon to significantly enhance NMR spectra and MRI images, which has revolutionized medical diagnostics technology. Ex-situ NMR or NMR without magnets is another technique developed in this program, which is expected to have an enormous impact on imaging in materials science, biology and medicine, and airport screening (humans and baggage) technologies.

Mission Relevance:

The research in this portfolio 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. Materials Chemistry and Biomolecular Materials program provides support for fundamental research in surface and interfacial chemistry, nanoscience, polymeric and organic materials, solid state chemistry, and development of new tools and techniques to advance the field of materials sciences. Research in these areas is at the forefront of the synthesis, assembly, and understanding of materials.

Scientific Challenges:

The major challenge in this core research activity is identifying and supporting the research focused on exploratory synthesis and discovery of new materials with novel properties that can lead to entirely new energy-related technologies. Developing experimental strategies for the “atom-by-atom” synthesis of materials with unprecedented nanoscale (and sub-nanoscale) structural control is clearly an outstanding challenge. In this context, a detailed understanding of hierarchical and dynamic self-assembly processes ubiquitous in nature can be an extremely valuable guide. Such a knowledge base can lead to low-temperature, energy-efficient synthesis routes to new materials and new manufacturing processes.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007
46,860	40,694	49,748

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Performers (FY2005)	Funding Percentage
DOE Laboratories	63%
Universities	35%
Other	2%

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:

In addition to maintaining a healthy core research activity, the program will further expand into nanoscience research, particularly at the nano-bio interface. It will seek to develop new multi-disciplinary approaches, with biology, chemistry, physics and computational science playing major roles, to model, design and synthesize new and novel materials. Some of the targeted areas that will receive support in the coming years include novel materials and innovative concepts that will impact solid state lighting, hydrogen production and storage, novel electrodes and membranes for improving the efficiency of fuel cells, and theory and modeling to aid new materials discovery. Also of particular interest is the development of new organic electronic materials with novel magnetic, conducting, and optical properties. The program will also facilitate multi-investigator, multi-disciplinary team research, to bring appropriate talents to bear on increasingly more complex and multi-functional materials. The program will continue to identify and support high-risk, high-impact, and often ground-breaking research.