Research Activity:	**Materials Chemistry and Biomolecular Materials**
Division:	Materials Sciences and Engineering
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Portfolio Description:

This activity supports basic, exploratory research on the design, synthesis, characterization, and properties of novel materials and structures. The general focus is on the chemical aspects of complex and collective phenomena that give rise to advanced materials. The portfolio emphasizes solid-state chemistry, surface and interfacial chemistry, and materials that underpin many energy-related areas such as fuel cells and batteries, catalysis, energy conversion and storage, friction and lubrication, light-weight and high-strength materials, membranes, luminescent materials, and materials aspects of environmental chemistry. It includes investigation of novel materials such as self-assembled structures, cluster and nanocrystal-based materials, quasicrystals, polymers, macromolecular assemblies and solids, superconductors, organic electronic and magnetic materials, porous materials, complex fluids, hybrid and composite materials and biomolecular materials. There is an increased emphasis on the synthesis of new materials with nanoscale structural control and taking advantage of unique material properties that originate at the nanoscale. Significant research opportunities also exist at the biology/materials science interface since the world of biology offers time-tested strategies and models for the design and synthesis of new materials – composites and molecular assemblies with unique properties and specifically designed functions. The program also supports the development of new experimental tools and techniques such as high-resolution magnetic resonance imaging (MRI) outside the magnet, x-ray and neutron reflectometry, time-resolved electron diffraction, optical and scanning probe microscopies for dynamic imaging, and surface force apparatus in combination with various spectroscopies.

Distinguishing Features:

To a large measure, the projects supported in this portfolio have a substantial emphasis on fundamental science and a significant "chemistry" component, which is invariably, coupled with physical and/or biological science components. Since new materials open up new possibilities and usher in new opportunities in energy-related technologies, there is considerable interest in the "discovery" of new materials, systems and properties. 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/LBNL), neutron reflectometers (Felcher/ANL and Russell/U. Mass), combinatorial materials chemistry for new materials discovery (Schultz/Scripps Research Institute), the surface force apparatus (Israelachvili/UC Santa Barbara and Steve Granick/UIUC), 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 Others:

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 National Labs 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 SC, NNSA, FE, EM, NEST and EE&RE.
- Programs PI's are collocated and occasionally co-funded by EE&RE (batteries and fuel cells, green chemistry, solar energy conversion, hydrogen storage), FE (catalysis and advanced materials research), and NNSA-DP (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 was initially formed to formulate 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 NSF and NIH through joint workshops and joint funding of select activities as appropriate (two currently active).
- Industrial interactions: 15 active CRADAs at four DOE laboratories.

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 it offers great promise for finding a non-platinum, direct fuel cell that uses organic liquids (methanol, ethanol etc.) as fuel (DiSalvo and Arbuna, 2003). A biomolecular route found in Nature has been harnessed to produce photovoltaic and semiconductor nanocrystals at low temperature and under environmentally benign conditions (Morse, 2003). A truly remarkable recent achievement is the generation of a bacterium with a 21amino acid genetic code, which can eventually lead to our ability to generate proteins with entirely new or enhanced biological functions (Schultz, 2003). 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:

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. 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, light-weight and high-strength materials, membranes, luminescent materials, and materials aspects of environmental chemistry.

Scientific Challenges:

The major challenge in this core research activity is identifying and supporting the research focused on 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.

Another major challenge is the development of new experimental techniques and tools for the detection, analysis and manipulation of materials, their structures and their properties.

Funding Summary:

Dollars in Thousands

FY 2003	FY 2004	FY 2005 request
40,563	42,000	44,437

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Performers	Funding Percentage
DOE Laboratories	71%
Universities	27%
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. Performers in FY2003 included 46 DOE Laboratory projects and 52 university grants. The 'Other' category includes a grant to a small company (Mission Support, Inc., in Utah) to develop new solid-state detectors for neutron scattering research and two projects supported jointly with the Division of Materials Research, NSF.

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. With the advent of advanced x-ray synchrotron and neutron facilities within the DOE complex, which are expected to provide new insights into the physics of advanced materials, e.g., superconductors, GMR and CMR materials, optical materials etc. there is a great demand for high-quality single crystals (and other forms) of such materials. Accordingly, there will be a new emphasis on single crystal growth of advanced materials, which will lead to better characterization, and consequently, better understanding of their properties. The program will also seek to facilitate multi-investigator, multi-disciplinary team research, to bring appropriate talents to bear on increasingly more complex and multi-functional materials. The program has sought to identify and support high-risk, high-impact and often ground-breaking research, and will continue to do so.