Research Activity:	**Materials Chemistry**
Division:	Materials Sciences and Engineering
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Division Director:	Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research in the development of novel materials and material constructs with an emphasis on synthetic 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, and molecular level understanding of friction, adhesion, and lubrication, and (5) development of new, science-driven, laboratory-based analytical tools and techniques.

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, where the emphasis is on physical control of structure and properties. Significant interactions and collaborations exist between the principal investigators in this activity and the X-Ray and Neutron Scattering activities 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 nanoscience, solid state NMR and MRI, organic magnets, organic conductors and superconductors, polymer composites, organic-inorganic hybrid 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, neutron reflectometers, combinatorial materials chemistry for new materials discovery, the surface force apparatus, and spin-polarized metastable helium scattering. 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, and engineering. This interfacing results in very active relationships.

- Within BES, there are jointly funded programs in the DOE national laboratories and universities, 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).
- Principal investigators are co-located and occasionally co-funded by EERE (batteries and fuel cells, green chemistry, solar energy conversion, and hydrogen storage), FE (catalytic materials 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 NSTC Nanoscale Science, Engineering, and Technology subcommittee (NSET), which formulated the National Nanotechnology Initiative (NNI). This subcommittee meets monthly to coordinate the NNI.
- Very active interactions with the National Science Foundation (NSF) through joint workshops and joint funding

of select activities as appropriate (two currently active).

Significant Accomplishments:

This activity is responsible for the discovery of the first organic magnet, the highest-T_c organic superconductor, the first all-organic superconductor, and the first room temperature organic magnet. 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. The first material that simultaneously exhibits bistability in three physical channels – electronic, magnetic, and optical – was discovered. 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. New combined experimental and theoretical work has demonstrated that semiconductor nanowires can be designed to achieve extremely large enhancements in thermoelectric efficiency, a factor of 100 for silicon, and that the temperature of maximum efficiency may be tuned by changing the dopant and the nanowire size. Theory indicates that similar improvements should be achievable for other semiconductor systems because of phonon effects. Another nanoscience accomplishment involves the discovery of a new, inherently inexpensive solution-based technique to synthesize one-dimensional "superlatticed" nanorods. Superlatticed refers to semiconductor structures with alternating layers of different compositions. Theoreticians in the multi-investigator group who achieved this predicted that as the composition of the superlattice was changed strain engineering would induce the spontaneous formation of one-dimensional materials and superlatticed structures with their predicted outstanding electronic and photonic properties playing a key role in devices.

This activity 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. This activity 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. Recent work by this group is the first application of gas phase MRI to microfluidic catalysis. They developed a technique in which parahydrogen-polarized gas is used to make an MRI signal strong enough to provide direct visualization of the gas-phase flow over active catalysts in packed-bed microreactors. These early results are expected to have significant effects on catalysis research in the near future.

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. The Materials Chemistry 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 materials characterization. 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. Realization of this challenge can lead to novel synthesis routes to new materials and new materials properties.

Funding Summary*:

Dollars in Thousands

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

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

* Represents combined total 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:

In addition to maintaining a healthy core research activity, the program will further expand into nanoscience research, with an emphasis on the discovery of new materials and strategies for solar energy conversion, hydrogen generation and storage, and electrical energy storage. It will seek to develop new multi-disciplinary approaches, with 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 also include novel materials and innovative concepts that will impact electrical energy storage, novel electrodes and membranes for improving the efficiency of fuel cells, and theory and modeling to aid new materials discovery. Also of interest is the development of new instrumentation to measure forces and other physical and chemical properties with ultrahigh sensitivity to further advance the nanoscale science. 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 strive to identify and support high-risk, high-impact, and often ground-breaking research.