Research Activity: **Materials Chemistry**

Division: Materials Sciences and Engineering

Primary Contact(s): Richard D. Kelley (Richard.Kelley@science.doe.gov 301-903-6051)
Aravinda M. Kini (Aravinda.Kini@science.doe.gov 301-903-3565)

Team Leader: William T. Oosterhuis

Division Director: Patricia Dehmer, Acting

Portfolio Description:

This activity broadly 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 batteries and fuel cells, catalysis, friction and lubrication, energy conversion and storage, membranes, electronics and sensors, and materials aspects of environmental chemistry. It includes investigation of novel materials such as low-dimensional solids, self-assembled monolayers, cluster and nanocrystal-based materials, conducting and electroluminescent polymers, organic superconductors and magnets, complex fluids, hybrid materials, biomolecular materials and solid-state neutron detectors. 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. In this regard, addition of a new Program Manager (A. M. K.) for Biomolecular Materials has added a new dimension to the scope of Materials Chemistry research activity. Significant research opportunities 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 specific functions. A wide variety of experimental techniques are employed to characterize these materials including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and x-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as high-resolution magnetic resonance imaging (MRI) without magnets, neutron reflectometry, and surface force apparatus in combination with various spectroscopies.

Unique Aspects:

Investigators 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 without magnets (Pines/LBNL), neutron reflectometers (Felcher/ANL and Russell/U. Mass), combinatorial 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. R. D. K. is currently the Chair of Electrochemical Technologies Subcommittee of EMaCC.
- 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 federal initiative.

- 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; Grant to a small business to develop solid-state neutron detectors.

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) and the first room temperature organic magnet (Miller and Epstein, 1991). This work 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 potentially new, enabling technologies. Very recently, the first material that simultaneously exhibits bistability in three channels – electronic, magnetic and optical – has been discovered (Haddon, 2002).

The program also pioneered the development and use of 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 a huge impact on imaging in materials science, biology and medicine, and airport screening (humans and baggage) technologies.

Mission Relevance:

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 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, friction and lubrication, membranes, sensors and electronics, and materials aspects of environmental chemistry. New techniques for the fabrication of nanocrystals have generated a unique inverse micellar process that makes possible the efficient elimination of dangerous chlorinated organic and phenolic pollutants (e.g., PCP). Similarly, the development of synthetic membranes using biological approaches may yield materials for advanced separations and energy storage. A new approach involving the use of ordered intermetallic materials as fuel cell electrodes offers great promise for finding a non-platinum, direct fuel cell that uses organic liquids as fuel (methanol, ethanol and other similar chemicals). Research on solid electrolytes is already paying off in new, very thin rechargeable batteries that can be recharged many more times than the present generation batteries. Research supported by this program on chemical vapor deposition (CVD) continues to have a great impact on the electronics industry.

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 2002	FY 2003 Request	FY 2004 Request
27,287	29,602	29,563

.

Performers	Funding Percentage
DOE Laboratories	74%
Universities	25%
Other	1%

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 FY2002 included 43 DOE Laboratory projects and 51 university grants. The 'Other' category includes a grant with a small company (Mission Support, Inc., in Utah) to develop new solid-state detectors for neutron scattering research and two projects supported jointly with 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. 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. Other areas that will receive support include solid state neutron detectors, high pressure synthetic chemistry, organic lasers and LEDs, polymer interfaces, and theory and modeling to help new materials discovery. 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.

February 27, 2003