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:	Iran L. Thomas

Portfolio Description:

This activity supports basic research on the synthesis, characterization, and chemical properties of materials to understand the effects of chemical reactivity on the synthesis and behavior of novel materials and structures. The portfolio emphasizes surface and interfacial chemistry, nanoscience, solid state chemistry, polymers, and organic materials that underpin many energy-related areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics and environmental chemistry. It includes investigations of novel materials including low-dimensional, self-assembled monolayers; cluster and nanocrystal-based materials; polymeric conductors; organic superconductors and magnets; complex fluids; biomolecular materials; and solid state neutron detectors. The research employs a wide variety of experimental techniques 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, atomic force microscopy of liquids, nanopatterning with self-assembly of block copolymers, and surface engineering of hybrid living/nonliving systems.

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, polymers, nanoscience, organic-inorganic composite materials, basic science of tribology, and advanced inorganic materials including quasicrystals.

Investigators in this program have conceived, developed, and exploited novel instrumentation/techniques such as high resolution MRI without magnets (Pines/LBNL), neutron reflectometers (Felcher/ANL and Russell/U. Mass), combinatorial chemistry for new material discovery (Schultz/LBNL (now Scripps Research Institute), the surface force apparatus (Israelachvili/UC Santa Barbara), and spin polarized metastable helium scattering (El-Batanouny/Boston University)

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 DP, EE, RE, FE, and EM; laboratory investigators collocated and occasionally co-funded by EE & RE (transportation technologies (batteries and fuel cells), industrial technologies (Green Chemistry), solar energy technologies (hydrogen storage), FE (catalysis and advanced materials research), and DP (nanoscience research).
- Within the federal agencies, the program coordinates through the Federal Interagency Chemistry Representatives (FICR), 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 initially was 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 with small business to develop solid state neutron detectors.

Significant Accomplishments:

This program is responsible for the discovery of the first organic magnet (1986) and the first room temperature organic magnet (1991). This work created a new field of research, which has grown substantially since these discoveries and has transformed organic magnets from an impossibility to a thriving new science and potentially new, enabling technologies. The program 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 in great demand. The program pioneered and developed the use of laser polarized xenon to significantly enhance NMR spectra and MRI images in materials science, in medicine, and in biology.

Mission Relevance:

Materials Chemistry 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 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 technological areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics, and environmental chemistry. New techniques for 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 synthesis may yield materials for separations and energy storage. Research on solid electrolytes is already paying off in new very thin rechargeable batteries that can be recharged many more times than existing commercial cells. Research on polymers may lead to lightweight structural materials that can be used in automobiles and thereby providing substantial savings in energy efficiency. Research in this program on chemical vapor deposition (CVD) continues to impact the electronics industry.

Scientific Challenges:

The increasing complexity and variety of materials offers many opportunities. The challenge is to choose the right directions from among the many combinations. The choices are expected to be abundant in nanoscale science where the “explosion” of exciting activity across a wide spectrum of scientific disciplines has brought about an interagency research initiative, National Nanotechnology Initiative. This initiative, to rapidly expand the ongoing research, will require many choices and the guidance of earlier and future workshops of experts and the peer review community.

Materials Chemistry research is needed to find new solid state materials for advanced neutron and x-ray detectors.

Experimental and theoretical research is needed to explore new approaches to the understanding of the origins of complex and cooperative phenomena in soft materials.

Funding Summary:

Dollars in Thousands

FY 2000	FY 2001	FY 2002
$25,353	$30,808	$27,823

.

Performer	Funding Percentage
DOE Laboratories	72.0%
Universities	25.0%
Other	3.0%

Performers in FY2001 included 37 DOE Laboratory projects and 45 university grants The ‘Other’ category includes a grant with a small company (Mission Support, Inc., in Utah) that is conducting research to develop new solid state detectors for neutron scattering research and two projects jointly supported with NSF.

Projected Evolution:

Beyond maintaining a healthy core research activity, the program will expand nanoscience research, particularly to explore new techniques with combination of biological, organic, inorganic, and physics approaches. Other areas that will receive additional support will include solid state neutron detectors, high pressure synthetic chemistry, organic lasers, polymer interfaces, and increased theoretical chemistry.

Increased emphasis on new synthetic routes to advanced materials including biologically-inspired, macromolecular, and composite materials and complex fluids research.

Increased multi-investigator, multi-disciplinary team research, to bring appropriate talent to bear on increasingly more complex materials chemistry.

04 February 2001