Research Activity: Theoretical Condensed Matter Physics

Division: Materials Sciences and Engineering
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Portfolio Description:

The Theoretical Condensed Matter Physics activity provides theoretical support for all parts of the Materials Science and Engineering Division. Research areas include quantum dots, nanotubes and their properties, tribology at the atomic level, superconductivity, magnetism, and optics. A significant part of the portfolio consists of the development of advanced computer simulation algorithms and fast codes to treat many-particle systems. An important component of the portfolio is the Computational Materials Science Network (CMSN), which brings together groups of scientists from DOE laboratories, universities, and (to a lesser extent) industry to solve materials problems requiring collaboration across disciplinary and organizational boundaries.

Unique Aspects:

The rapid advance in technological and computational capabilities makes it possible to perform research in condensed matter theory and materials science at an unprecedented level of sophistication. The resulting complexity of the research requires an increasing diversity of disciplines. Consistent with the increasing acceptance of computational science as a “third way of doing science” the activity includes the Computational Materials Science Network. The CMSN is a unique program that brings together a multi-disciplinary group of scientists from DOE laboratories, universities, and industry to collaborate on computational materials science projects. At present CMSN consists of five sub-projects: Excited State Response Functions (testing the accuracy of current levels of fundamental theory); Microstructural Effects on the Mechanics of Materials (computational study of the fundamental basics of metallurgy); Microstructural Evolution Based on Fundamental Interfacial Properties (a fundamental factor to understand the processing of real materials); Polymers at Interfaces (a study of failure modes since this region is the weakest link in composite materials); Magnetic Materials Bridging Basic and Applied Science (an attempt to interconnect different scales of magnetic behavior from quantum mechanical electronic behavior al the way to continuum micro-mechanical properties). Other projects will be considered including electronic structure techniques tailored specifically to nanoparticles, polymer matrixing, and complex correlation issues.

Relationship to Others:

Within DOE a high level of collaboration exists between MICS and NERSC. Information on university grants is shared with NSF, peer reviews are sometimes shared, and on occasion there is joint funding of grants. On the international level participation in organizing and steering committees is frequent, as are exchanges of experts between foreign and domestic institutions.

Significant Accomplishments:

Consistent with the emphasis on nanoscience enabled by developments in technology and computational techniques, notable achievements in this area have been made within the Condensed Matter Theory Activity.
Research into low dimensional materials has revealed exciting new information and has pointed to new possibilities in creating new tailored materials and devices. Highlights include:

1. The discovery that magnetization around defects in quasi-one dimensional materials greatly influences the phase in which they reside points to the development of sensors highly sensitive to external stimuli.
2. The discovery that loading electrons into quantum dots results in the formation, within the dot, of complexes of holes and electrons. These decay in a theoretically predictable manner, pointing to the possibility of fabricating quantum dots with tailored light emitting properties.
3. The discovery that electrons confined in a thin film segregate into discreet energy levels, in analogy to the discreet energy levels in atoms, points to the possibility of constructing ultra-stable materials by controlling the thickness of the film.

4. Calculations show that the conductance across two crossed carbon nanotubes is very sensitive to the force applied at that junction. While the inter-tube conductance is dramatically increased, the intra-tube conductance is diminished. When this arrangement is realized experimentally, crossed nanotubes can be expected to be excellent sensors for applied forces within nanoscaled devices.

Significant progress has also been made in other areas as illustrated by the following examples.

Dynamic mean-field theory, which is exact for infinite dimensions, has been successfully coupled with three dimensional band theory. The resulting hybrid theory predicts the anomalous properties of highly correlated rare-earth and actinide materials.

When metals solidify they form highly branched patterns called dendrites. These solidification patterns control many aspects of processing and microstructure and hence our ability to use materials. A Collaborative Research Team of the Computational Materials Science Network has devised an entirely new method for extracting the anisotropy of energy and mobility responsible for dendrite formation from supercomputer simulations of the atomic processes occurring during solidification.

Ab initio calculations have been performed for the hysteresis loop and domain wall dynamics of magnets. Long thought to be beyond the scope of *ab initio* calculations because of the large number of atoms involved, it became possible to perform detailed studies of some less demanding materials such as FePt and CoPt, which are technologically important.

Mission Relevance:

The program's ultimate purpose is to understand the properties of existing materials and to create new ones that are more efficient in producing, storing, and using energy. To this end, the programs in this portfolio have the common goal of achieving a basic understanding of matter ranging from the atomic to the bulk scales. The experimental and theoretical programs work in close collaboration with each other, but more independent modes of research also exist. Theorists will try to establish a theoretical basis for experimentally observed results, which almost always suggests further experiments, and thus leads to new results. New science is produced by simulating processes on computers, "computer experiments" which are difficult or impossible perform in the laboratory. The behavior of the surface layers of materials sliding on each other and a new understanding of the role of lubricants has been obtained in this way. Other examples include investigations into the behavior of electrons flowing in nano wires and nanotubes and in the properties of matter at extreme conditions of temperature and pressure.

Scientific Challenges:

Because of the close relationship between the experimental and theoretical elements, many of these are common to both. Examples of areas common to both are exploring the behavior of complex systems, investigating nano-scale systems, and understanding superconductivity. In theory, the need to develop functionals defined by the Density Functional Theory and needed for its applications is an example as is the need to develop more efficient algorithms for the efficient use of modern computers.

Funding Summary:

Dollars in Thousands

FY 2000	FY 2001	FY 2002
$14,888	$16,124	$18,116

Performer	Funding Percentage
DOE Laboratories	79.0%
Universities	21.0%

The program provides funding for 47 university grants supporting about as many students and partially supporting about 50 faculty and senior staff and programs at 9 national laboratories. There are approximately 70 postdocs fully or partially supported by this CRA. Programs at the laboratories are multi-investigator efforts on problems that require extensive participation experimental and theoretical scientists. This program supports research at LBNL, AMES, BNL, ANL, LLNL, MRS, LANL, ORNL, and NREL. Many of the research efforts at national laboratories involve interfaces with the university and industrial communities and user facilities. In addition, about $1.4M on is provided to projects of the Computational Materials Science Network.

Projected Evolution:

Rapid advancements in computer hardware and software will be exploited to model materials with ever-greater sophistication and realism. The ability to perform experiments at the nanoscale and similar advances in computational technology (software and hardware) has opened a new era in materials science. It is expected that increasing emphasis will be placed on nanoscience studies. For the theory program, this will necessitate an even tighter coupling between theory and experiment.

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