**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 effort within the portfolio is the development of advanced computer algorithms and fast codes to treat many-particle systems. An important facilitating component is the Computational Materials Science Network (CMSN), which enables groups of scientists from DOE laboratories, universities, and (to a lesser extent) industry to address materials problems requiring larger-scale collaboration across disciplinary and organizational boundaries.

## Unique Aspects:

New areas of materials science are being identified and studied. New technology is enabling a much closer examination of the existing ones. This healthy progress dictates that new theories be developed and that established ones be reexamined and possibly extended. A very important contribution of the theorist is enforcing a rational, consistent understanding of experimental observations so that we can go forward. Often, this involves working out the implications of a theory for a specific material or situation. In materials, this can be an extremely difficult task because of the very many atoms involved. Many conceptual tools such as quasiparticles, entities defined to examine phenomena at different length scales, or summary statistical approaches have been developed. Further development of such conceptual tools continues to be a very important aspect of this theoretical program. However, for many phenomena now being studied, large scale computation must be utilized to perform the complex calculations involved or to perform the simulations of many interacting components. The rapid advance in computational capabilities now enables research at such a level of sophistication that computational science has become a "third way of doing science", but at a price. The complexity of such research very often requires larger groups of collaborating researchers from a diversity of disciplines. One response has been formation of the Computational Materials Science Network to bring together multi-disciplinary groups of scientists from DOE laboratories, universities, and industry to collaborate on computational materials science projects. At present, CMSN consists of five sub-projects: Excited States and 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 all the way to continuum micro-mechanical properties).

## Relationship to Others:

This activity interacts with all the other research activities within the Division of Materials Science and Engineering driven by mutual interest Also, because the computational resources at the National Energy Research Scientific Computing facility utilized by the division are administered here, there is an enhanced awareness of opportunity. Within DOE, frequent interaction occurs with the Mathematics, Information and Computer Sciences division. 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. 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.

When atomic motions within a material are simulated by molecular dynamics, much of the computational effort is expended to describe the rapid vibrations of the atoms about their equilibrium positions. This expenditure precludes running the simulation for long enough times to see a significant number of jumps of atoms between equilibrium positions --- the interesting phenomena in this case. To deal with this problem, a modified or hyper dynamics was developed that damps the rapid oscillations while accurately representing the site to site jumps. This greatly facilitates our ability to calculate atomic diffusion in materials.

## Mission Relevance:

The program's ultimate purpose is to understand the properties of existing materials and to reveal 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 at all scales ranging all the way from the atomic to the bulk. The experimental and theoretical programs work closely together, but there are also more independent modes of research. The theorists will try to establish a theoretical basis for experimentally observed results, which almost always suggests further experiments, and thus leads to new results. But new science is also produced by simulating processes on computers. "Computer experiments" can be performed which are difficult or impossible perform in the laboratory. They are also much easier to dissect and vary to determine the effective mechanisms. For example, 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:

The close relationship between the experimental and theoretical programs dictates that many challenges are common to both. Examples are exploring the behavior of complex systems, investigating nano-scale systems, and understanding superconductivity. New ways of conceptually visualizing and characterizing phenomena will broaden our horizons. Stripes occurring in cuprate superconductors and two dimensional electron gasses are an excellent example. Bridging length scales is a major thrust. The tactic of dividing up the effects in materials according to the length scale at which they occur has greatly facilitated our understanding. But for the theorists, this

creates the problem of how to pass needed information between the different constructs used at the different length scales. Only in that way can one calculate parameters rather than make phenomenological fits. Such is the basis for improved understanding and greater precision of our modeling. It is a continuing major goal on which limited progress has been made. Bridging time scales is similarly important but far less progress has been made. Basic theory improvements are also needed. For example, density functional theory is our most computationally tractable many body theory but it defines many functionals both for the ground state or ensemble energy and separately for the properties that must be determined. Whereas knowledge of the exchange-correlation functional for the ground state energy is reasonably advanced, knowledge of all other functionals is still quite rudimentary. Improvements are also needed in our computational tools. Materials theory is a very heavy consumer of computer resources even if not so visibly as in other disciplines. (This is because materials theory deals with many dissimilar problems rather than a few overarching ones.) The materials community could very productively make use of vast increases in computational capability. Because the phenomenal growth due to hardware improvements is actually overshadowed by those due to clever algorithm design, further improvements in "tool development" will significantly impact future development in a qualitative way.

## Funding Summary:

**Dollars in Thousands**

| FY 2002 | FY 2003 Request | FY 2004 Request |
|---|---|---|
| 18,007 | 18,007 | 17,982 |

| Performer | Funding Percentage |
|---|---|
| DOE Laboratories | 75% |
| Universities | 25% |

The program provides funding for 48 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 by 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 is provided to projects of the Computational Materials Science Network.

## Projected Evolution:

Materials will be modeled with ever-greater sophistication and realism and complexity. Needs and opportunities will drive the effort inexorably in this direction. Science at the nanoscale will continue a major example, although it is only one of many. With the Chemistry Division, a cooperative effort will be begun with Mathematics, Information, and Computer Sciences seeking to enhance our capabilities to model and simulate at the nanoscale. As a way to bring together teams adequate to address the more complex problems envisioned, the Computational Materials Science Network will be enhanced.