Research Activity: Theoretical Condensed Matter Physics

Division: Materials Sciences and Engineering
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Portfolio Description:

The Theoretical Condensed Matter Physics activity includes a broad spectrum of theoretically research complementing all parts of the Materials Science and Engineering Division. Research areas include structure and properties of quantum dots and nanotubes, two dimensional electron gas, quantum transport, tribology at the atomic level, superconductivity, magnetism, and optics. A significant effort within the portfolio is the development of advanced computer algorithms 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 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 dictated by the fundamental theory or to perform the simulations of systems with 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 assemble 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); Fundamentals of Dirty Interfaces: From Atoms to Alloy Microstructures (the development of microstructure in heterogeneous 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); Predictive Capability for Strongly Correlated Systems (an attempt to advance capabilities in many body theory).

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. By judiciously attaching molecules to nanoclusters, one can guide them to assemble in a specified manner. (The rule book remains to be written but it is under construction.)
2. Gold nanoparticles behave much more like their platinum group neighbors in the periodic table including exhibiting interesting catalytic behavior. When passivated by dodecane thiols, they can self-assemble into nanocrystalline superlattices with unique properties.
3. Nanocrystalline diamond can form with a bucky-ball-like surface reconstruction. The carbon nanoparticles exhibit very weak quantum confinement unlike silicon and germanium.
4. Silicon nanotubes can be formed by stabilization with a core of nickel atoms. Unlike carbon, silicon nanotubes are not stable without such help.

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 has been used to elucidate the spin polarization of CrO_2 --- a famous magnetic recording material that might find new use is spintronics. A competition between quasiparticle behavior and local –moment behavior is found.

A way has been found to see diffraction data for molecules adsorbed on surfaces. The conventional methods of low energy electron diffraction will not work: the molecules produce no Bragg spots because they are randomly distributed on the surface. However, it has been shown that the information is present in the intensity variation of the spots originating from the substrate. The resulting technique has successfully revealed the geometry of small hydrocarbons on a palladium surface.

The origin of the light-induced conductivity in the transparent oxide $12CaO{\cdot}7Al_2O_3$ is traced to electrons excited off H ions present. To accomplish this, it was first necessary to accomplish calculating the Coulomb gap leading to hopping conductivity.

Progress has been made on the question of how to treat core-hole effects in x-ray absorption spectra by a collaboratory research team of the Computational Materials Science Network. The team, which focuses on Excited States and Response Functions, brought together experts of all applicable approaches to compare against each other and elucidate the formal relationships between them. What resulted was an excellent prescription for success but with identified places for improvement. This is needed not only for fundamental understanding of the details of x-ray absorption phenomena but technological applications --- an example of which is the measurement of the thickness of integrated circuit interconnects.

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 try to establish a theoretical basis for experimentally observed results, which almost always suggests further experiments, and thus leads to new results. New experiments and experimental techniques are often suggested. 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 to vary the conditions in order to isolate 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. Other many body approaches, although far more computationally intensive, provide important information and require further development. Improvements are also needed in our computational tools. Materials theory is a very heavy consumer of computer resources even if not so visibly as 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 of science in a qualitative way.

Funding Summary:

Dollars in Thousands

FY 2003	FY 2004	FY 2005 Request
16,993	17,000	17,975

Performer	Funding Percentage
DOE Laboratories	75%
Universities	25%

The program provides funding for 54 university grants supporting about as many students and partially supporting about 60 faculty and senior staff. There are approximately 70 postdocs fully or partially supported by this CRA. This program supports research at LBNL, AMES, BNL, ANL, LLNL, MRS, LANL, ORNL, and NREL. Programs at the laboratories are multi-investigator efforts on problems that require extensive participation by experimental and theoretical scientists. Many of the research efforts at national laboratories involve interfaces with the university and industrial communities and with user facilities. Additionally, about $1.4M is provided for 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.