

Theoretical Condensed Matter Physics

Portfolio Description

This activity supports Theoretical Condensed Matter Physics with emphasis on the theory, modeling, and simulation of electronic correlations. A major thrust is nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other major research areas include strongly correlated electron systems, quantum transport, superconductivity, magnetism, and optics. Development of theory targeted at aiding experimental technique design and interpretation of experimental results is also emphasized. This activity supports the Computational Materials Science Network, which forms collaborating teams from diverse disciplines to address the increasing complexity of many current research issues. The activity also supports large-scale computation to perform complex calculations dictated by fundamental theory or to perform complex system simulations with joint funding from DOE's Advanced Scientific Computing Research program. Capital equipment funding will be provided for items such as computer workstations and clusters.

Unique Aspects

Research in condensed matter and materials science is intrinsically rich, not only because atoms and molecules can be assembled to produce an almost endless variety of materials, but also because we believe that there is a rational basis for complexity and emergent behavior, which derives from a few elegant laws of nature. There are three fundamental components to the program. First, theorists, working with awareness of challenges and discoveries from the experimental realm, are asked to advance the conceptual basis of our science in the form of analytic, predicable, quantifiable and verifiable theories. The second component is characterized by theoretical efforts motivated by the need to understand experimental observations. Answering why certain phenomena occur does not require new theory as often as it requires new insight. The third component involves the important role of computational tools and high performance computing. This program encourages researchers who employ computational approaches to advance science through the coupling of deep scientific insights, strong traditional theoretical talents, and creative use of computational resources. This includes working synergistically with other programs in BES where support of theoretical, computational and modeling efforts advances their programmatic focus.

Relationship to Other Programs

This activity is aggressive in maintaining interactions with other research activities within the BES, driven by the opportunity of stimulating theory through experimental discovery and bringing solid theoretical foundations and understanding to new processes of interest to experimental and facilities programs. Because this program has oversight responsibility for a portion of the supercomputer resources at the National Energy Research Supercomputer Center, there is particular interest in opportunities for implementing complex theoretical methods as predictive tools in support of experimental science and the broader community. Nanoscience-related projects are coordinated with the Nanoscale Science Research Center activities and are reviewed in the BES Scientific User Facilities Division. BES further coordinates the nanoscience activities with other federal agencies by participating in the National Science and Technology Council's Nanoscale Science, Engineering, and Technology subcommittee, which leads the

National Nanotechnology Initiative. The program also takes advantage of opportunities to collaborate with the Office of Advanced Scientific Computing Research. The BES commitment to advancing the frontiers of basic research is present in programmatic interactions with other programs in DOE such as the Office of Energy Efficiency and Renewable Energy and other Federal Agencies. Communication of ongoing research programs and goals is part of the interaction with the National Science Foundation and other agencies.

Significant Accomplishments

Consistent with an emphasis on nanoscale theory, notable advances through theory and modeling provide exciting new information and point to new possibilities for creating new tailored materials and devices. Highlights include:

- Functional nanoparticles have become the key to control and self-assembly. By judiciously modifying nanoclusters, one can guide them to assemble in a specified manner.
- Researchers have significantly enhanced our ability to simulate large scale (billion atom) clusters including electronic degrees of freedom and thus achieve *ab initio* predictive capability with wide application.
- Electronic properties of quantum dots can be predicted based on realistic materials.

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

- Dynamical Mean Field Theory offers a practical way to treat the correlations which dominate the properties of many correlated electron systems.
- Progress has been made on the question of how to treat core-hole effects in x-ray absorption spectra by a collaborative research team of the Computational Materials Science network.
- A new level of accuracy and reliability of excited state properties of materials has become possible with advances in Density Functional Theory.
- Transport in nanoscale systems now has some fundamental theoretical basis and computational implementations. A breakthrough in single molecule electronics is near.
- Spintronics is evolving quickly, with the recent years seeing a shift from simplistic to realistic materials models.

Mission Relevance

This activity provides the fundamental knowledge for predicting the reliability and lifetime of energy use and conversion approaches and develops opportunities for next generation energy technology. Specific examples include inverse design of compound semiconductors for unprecedented solar photovoltaic conversion efficiency, solid-state approaches to improving capacity and kinetics of hydrogen storage, and ion transport mechanisms for fuel cell applications.

Scientific Challenges

Many fundamental aspects of condensed matter and materials science are far from being understood. Beyond high temperature superconductivity, there are continuing discoveries of complex phase behavior of correlated electronic materials, and even more remains to be discovered related to their dynamics and nonequilibrium processes. Similarly, complex

materials, whether hard, soft or in the growing wealth of metamaterials, offer many opportunities for study of complex systems and emergent behavior.

Bridging length scales is a continuing major goal on which progress is ongoing. More than integrating atomic level scales with nanometer or mesoscales in materials, this also requires integrating the domain of quantum laws with classical laws of physics. Bridging time scales is similarly important with some of the most exciting advances coming now with new theoretical methods implemented in a computational environment. Basic theory has challenges. For example, density functional theory is moving to a resolution of the longstanding problems of correctly treating excited states. Treatment of non-equilibrium systems needs advances in non-equilibrium statistical mechanics. In the computational area, a variety of algorithms no longer scale to the tens of thousands of processors available now and will be faced with millions of processors in the future.

Projected Evolution

The program will continue to emphasize the development of our understanding of matter on the atomic scale and expanding to add the capability of addressing length scales both larger and smaller than the nanoscale is part of the scientific future of theory, modeling and simulation for condensed matter and materials. A rich future exists in basic science and applications surrounding highly correlated materials as well as novel superconductors. This research is motivated by the newest science of materials, as well as by the potential for impact on longstanding problems for energy technologies and for fundamental physics, including understanding of the physics of microstructure and granular material. Computationally enabled science is simultaneously growing in maturity and seeing dramatic advances. Those advances, which further the basic research and mission of BES, have a natural home in this program.