Theoretical Condensed Matter Physics

Portfolio Description

This activity supports Theoretical Condensed Matter Physics with emphasis on the theory, modeling, and simulation of electronic correlations. Major research areas include correlated electron systems, quantum phase transitions, magnetism, superconductivity, optical response, thermoelectric materials, and neutron and photon scattering. Research into fundamental material properties related to new or existing energy technologies, and theory targeted at aiding experimental technique design and interpretation of experimental results is also supported. The program includes modeling and simulation efforts in support of the interagency Materials Genome Initiative and research utilizing large scale computational science with joint funding from DOE's Advanced Scientific Computing Research (ASCR) program. Nanoscale and multi-scale modeling, as well as modeling at the mesoscale, are included.

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 there is likely 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 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. The Materials Genome Initiative has added a component of *validated* theory and modeling which includes data repositories aimed at increasing the rate of materials discovery. 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.

- Within BES, this research activity sponsors – jointly with other core research activities and the Energy Frontier Research Centers program, as appropriate – program reviews, contractor meetings, and programmatic workshops.
- The program actively collaborates with ACSR on research opportunities in large scale, advanced computational tools and resources.

- The BES commitment to advancing the frontiers of basic research is present in programmatic interactions with other DOE programs such as the Office of Energy Efficiency and Renewable Energy.
- Nanoscience-related projects are coordinated with the Nanoscience Research Center activities and reviews in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology subcommittee, which leads the National Nanotechnology Initiative.
- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the NSTC Subcommittee on the Materials Genome Initiative.
- Active interactions with the National Science Foundation through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.

Significant Accomplishments

The program has history of theoretical and computational advances which have contributed to the broad understanding of condensed matter physics. Examples are the so-called GW method which provided a first principles theory of the bandgap of semiconductors such as silicon, the prediction of topological insulators, the theory and design of photonic band gap materials, the development of software to predict x-ray absorption in materials and its use to obtain atomic geometry, the understanding of the critical role of vortices in superconductors, the prediction of the intensity optical absorption in semiconducting nanoparticles, and for advances in dynamical mean field theory, a widely used method for treating correlated electron materials, and its use to understand neutron scattering in actinides. Recent accomplishments include:

- Development of an accurate computational approach to the theory of excitons in semiconductors;
- A new strategy for increasing the magnetic field from superconducting magnets through vortex pinning; and
- Better understanding of the role of quantum phase transitions in high temperature superconductivity.

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 the nanometer or mesoscale 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 theory and computation which extend the understanding of strongly correlated materials including magnetic and superconducting materials and transition metal oxides. There is a growing interest in exotic states of matter such as the quantum Hall effect and topological insulators. Predictive theory and modeling as it relates to the Materials Genome Initiative will become more important, as will advanced computational techniques such as the Quantum Monte Carlo method. Time dependent and non-equilibrium phenomena, especially at the femtosecond time scale and in electron transport are important areas for future research. All of these have the potential to impact energy relevant technologies over the long term.