

Theoretical Condensed Matter Physics

Portfolio Description

This program supports research in Theoretical Condensed Matter Physics with an emphasis on quantum materials, materials discovery, non-equilibrium transport and ultrafast response, and fundamental research in materials related to energy technologies. Suitable topics include strongly correlated electron systems, quantum phase transitions, magnetism, superconductivity, semiconductors, thermoelectric materials, optical response, neutron and photon scattering, theory of nanoscale and mesoscale systems, and computational and data-driven materials design. Approaches from purely analytical to computational are supported, as are methods that incorporate multiple length and time scales. Computational materials research may include development of validated, open-source codes and data analytics.

Scientific Challenges

The Theoretical Condensed Matter Physics activity explores and advances the frontiers in research through the application of the methods and principles of physics. Doing so requires addressing specific scientific challenges and opportunities, such as those identified in the BES reports: *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*, *From Quanta to the Continuum: Opportunities for Mesoscale Science*, *Computational Materials Science and Chemistry*, and *Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology* (<http://science.energy.gov/bes/community-resources/reports/>).

Challenges and opportunities identified in these reports include research on high-temperature superconductivity and beyond, where continuing discoveries of complex phase behavior remain to be understood and related to their dynamics and non-equilibrium processes. Similarly, complex materials offer many opportunities for the study of quantum 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 from new theoretical methods implemented in a computational environment. Basic theory has challenges; for example, density functional theory is moving to a resolution of the long-standing problems of correlations and for 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 that extend the understanding of quantum materials. These include strongly correlated materials, magnetic and superconducting materials, and transition metal oxides with targeted quantum properties, as well as exotic states of matter, for example those found in topological insulators, as well as Dirac and Weyl semimetals. The BES Basic Research Needs workshop report on *Quantum Materials for Energy*

Relevant Technology identified related topics. 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 for predictive materials science. Time-dependent and non-equilibrium phenomena, especially at the femtosecond time scale and in electron transport, are important areas for future research.

Cold atom, soft matter and biomolecular physics, polymers, glassy systems, granular materials, ionic liquids, surface chemistry, and quantum computing are not current priorities in Theoretical Condensed Matter Physics.

Significant Accomplishments

The program has a history of enabling theoretical and computational advances that have contributed to the broad understanding of condensed matter physics. Examples include many-body perturbation theory as implemented in the GW method, which provided a first-principles theory of the band gap of semiconductors; 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 dissipation of vortices in superconductors; the prediction of the intensity of optical absorption in semiconducting nanoparticles; and 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:

- Prediction of new topological states in materials including Dirac and Weyl semi-metals.
- Development of high throughput computational techniques for materials discovery including the Materials Project—an open database with more than 65,000 inorganic compounds and the largest collection of calculated elastic tensors.
- Improved quantum Monte Carlo techniques for strongly correlated materials including the ability to treat spin-orbit interactions.
- Methodological advances of the local density approximation combined with the Gutzwiller approximation to determine the structural properties of strongly correlated electron materials, including finite temperature effects.
- Microscopic model of silicon nanowire to help explain the voltage-tunable circular photogalvanic effect, i.e., a photocurrent with direction determined by the chirality of light.

Unique Aspects

Research in predictive theory and modeling has an emphasis on functional materials, excited states, and high-throughput computation. Novel, physics-based computational techniques are supported including quantum Monte Carlo, improvements to density functional theory, extensions of dynamical mean field theory, density matrix renormalization group, and self-consistent GW calculations (calculations based on many body perturbation theory which includes electron-electron and electron-hole interactions). The program will continue to emphasize basic research on matter at atomistic length scales, expanding to include properties at the mesoscale. Research supported by this program is motivated by recent developments in materials science, advancing the understanding of fundamental physics, and the potential for impact on energy technologies.

A unique component of this program is the support of theoretical efforts to understand experimental observations. This includes theory extracting basic physical insights from experiments at national scientific user facilities, such as the x-ray free electron laser at SLAC National Accelerator Laboratory, synchrotron light sources, and the Spallation Neutron Source.

Mission Relevance

The Theoretical Condensed Matter Physics program supports fundamental research on the principles of physics to understand, predict, and ultimately control matter and energy at the level of electrons, atoms, and molecules. This research provides the foundation for new materials that will underpin the future development of energy-relevant technologies including systems for energy storage, transformation, and utilization, with levels of performance superior to the current state of the art.

Relationship to Other Programs

This program maintains strong 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 program includes modeling and simulation efforts in support of the interagency Materials Genome Initiative (MGI) and research utilizing large-scale computational science with joint funding from DOE's Advanced Scientific Computing Research (ASCR) program. The MGI 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 high-performance computing resources at the National Energy Research Supercomputer Center (NERSC), 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 BES core research activities as appropriate—program reviews, principal investigators' (PI) meetings, and programmatic workshops.
- These research efforts are closely coordinated with other core research activities in BES, including Experimental Condensed Matter Physics on superconductors, nanostructures, and low-dimensional systems.
- The program actively collaborates with ASCR on research opportunities in large-scale, advanced computational tools and resources through the Scientific Discovery through Advanced Computing (SciDAC) partnership.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center activities in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Nanotechnology Coordination Office, which provides technical and administrative support to the National Science and Technology Council (NSTC) Subcommittee on Nanoscale Science, Engineering, and Technology for 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 (MGI).

- There are particularly active interactions with the National Science Foundation through the MGI PI meetings, workshops, and communication about research activities.