Physical Behavior of Materials

Portfolio Description

This activity supports basic research on the physical behavior of materials in response to electric fields, magnetic fields, electromagnetic fields, chemical environments, thermal excitation, size effects, and the proximity effects of surfaces and interfaces. Emphasis is on developing a fundamental understanding of processes taking place between charge carriers, photons, lattice vibrations, and other collective excitations in materials. Included within the activity is research to understand the role of crystal defects, phase equilibria and kinetics of reactions in materials in unusual environments, and diffusion and transport phenomena encountered in energy applications.

Scientific Challenges

The challenge in this area is to develop the scientific understanding of the mechanisms that control the behavior of materials and to use that understanding to design new materials with desired behaviors. The program encompasses efforts aimed at understanding the behavior of organic and inorganic electronic materials, magnetism and advanced magnetic materials, manipulation of light/photonic lattices, corrosion/electrochemical reactions, and high-temperature materials behavior through intimately connected experimental, theoretical, and modeling efforts leading to *a priori* design of new materials.

Specific scientific challenges and opportunities are identified by the BES Advisory Committee's reports (https://science.energy.gov/bes/community-resources/reports/), including *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* and *From Quanta to the Continuum: Opportunities for Mesoscale Science,* as well as the BES Basic Research Needs workshops.

Projected Evolution

The long-term goal of this program is to develop an atomistic understanding of the macroscopic physical behavior of materials. It is important to understand the relationship between a material's properties and its response to external stimuli. This can be achieved by determining structure-property relationships over multiple length scales, with emphasis at the atomic level, and by understanding the response of the nanometer and mesoscale features of the material to those external stimuli. This program seeks to foster theory, modeling, and simulation activities that address charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics in energy relevant materials.

The program currently emphasizes electronic and magnetic behavior of materials. The program also supports corrosion and electrochemistry science, nanoscale phenomena, and multiscale modeling of materials behaviors. Increased investment in photon-matter interactions and plasmonics will be considered. In addition, research that is focused on theory and modeling of physical behavior of materials, especially in the area of defects in crystals and their influence on the structural properties of materials will be deemphasized.

Significant Accomplishments

This activity has had broad and significant impact in many classes of materials and phenomena.

Some of the recent accomplishments include:

- Invention of world's smallest transistor with 1-nanometer gate lengths using MoS_2 material, and a one-nanometer diameter single walled carbon nanotube as a gate electrode, achieving near ideal operational characteristics of a transistor.
- Discovery of near-unity photoluminescence quantum yield in MoS_2 material, achieved by a special surface treatment they developed, increasing the room temperature photoluminescence quantum yield from 0.6% to 95%. The treatment eliminates defect-mediated nonradiative recombination, yielding near-perfect properties that opens the door for the development of highly efficient light-emitting diodes, lasers, and solar cells based on two-dimensional (2D) materials.
- Discovery of thermally injected spin current in a metal that can be amplified 10-fold, when a one-nanometer thick antiferromagnetic layer (like NiO or CoO) is introduced between the source (Yttrium Iron Garnet) and the metal.
- Discovery of the first 2D material that supports both superconducting and topological states at the same time. Researcher demonstrated by first-principles theory, scanning tunneling spectroscopy, and angle-resolved photoemission spectroscopy that the (2D) superconductor of single-layer FeSe also exhibits one-dimensional topological edge states.
- Discovery of an anomalously low electronic thermal conductivity in metallic VO_2 material at temperatures above room temperature. Such anomalies where charge carriers not contributing to the heat conduction in materials has only been observed at extremely low temperatures before.
- Discovery of a $B_{12}(CN)_{12}^{2-}$ molecule with colossal stability that may find potential use as a halogen-free electrolyte in batteries. State-of-the-art theoretical modelling studies discovered that CN ligand substitution for hydrogen in $B_{12}H_{12}^{2-}$ increases the second electron binding energy from 0.9 eV to 5.3 eV and makes it an extremely stable molecule.

Unique Aspects

This program supports research to develop a fundamental understanding and identification of detailed mechanisms responsible for the physical behavior of materials, and the incorporation of this knowledge into predictive models. Unique activities of the program include the design and characterization of new materials and the manner in which they interact with electromagnetic fields. These range from photo-induced charge transport in novel semiconducting materials to the optical interactions with meta-materials resulting in phenomena that could not be observed in naturally occurring materials. The research supported includes investigations on novel methods to modify the bandgap energy of materials for photovoltaics and optoelectronics. The program also emphasizes research to understand influence of magnetic fields on materials. Within BES, the program uniquely supports research on the thermal behavior of materials, investigating thermoelectric and magnetocaloric effects.

Mission Relevance

The research supported by this activity is necessary for the discovery of novel material properties and improving materials performance and reliability in chemical, electrical, and electrochemical applications, including the ability to generate and store energy in materials. Materials in energy-relevant environments are increasingly being exposed to extreme temperatures, strong magnetic fields, and hostile chemical conditions. A detailed understanding of how the physical-properties behavior of materials is linked to these surroundings and this exposure history is critical to the

understanding of photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, corrosion, novel magnetic materials for low-magnetic-loss power generation, magnetocaloric materials for high-efficiency refrigeration, and new materials for high-temperature gasification.

Relationship to Other Programs

This activity closely interacts with other programs in BES as well as with other DOE activities and interagency coordination groups:

- Within BES, this research activity sponsors—jointly with other core research activities, the Energy Frontier Research Centers program, and the Joint Center for Energy Storage Research (JCESR), as appropriate—program reviews, principal investigators' (PI) meetings, and programmatic workshops.
- There are active interactions with the DOE Office of Energy Efficiency and Renewable Energy (EERE) through workshops, program reviews, PI meetings, and communication of research activities and highlights.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center activities and reviews in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Nanotechnology Coordinating Office (NNCO), which provides technical and administrative support to the National Science and Technology Council (NSTC) Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) for the National Nanotechnology Initiative (NNI).
- 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).
- The program also participates in interagency coordination groups such as the Interagency Coordination Committee on Hydrogen and the Federal Interagency Materials Representatives (FIMaR).
- There are particularly active interactions with the National Science Foundation (NSF) through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.