

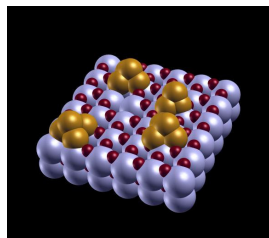
CENTER FOR COMPUTATIONAL MATERIALS SCIENCE

- The Center for Computational Materials Science is part of the Naval Research Laboratory. We conduct research on the electronic, structural, and mechanical properties of diverse materials systems including metals, semiconductors, and insulators in ordered and disordered states and in alloys and compounds. Both computational and analytical techniques are used to study the properties of condensed-matter and atomic/molecular systems.
- Major current research directions include new computational methods, disordered systems, energy storage and generation, thin films, magnetic materials, molecules and clusters, mechanical properties, nanostructures, quantum computing, quantum dots, radiation in matter, superconductivity, and surface science.
- A wide variety of computational methods are used, including first-principles electronic-structure methods, numerical statistical-mechanical methods, quantum many-body theory, and density-matrix approaches. Supercomputers and a variety of visualization techniques are utilized to make direct comparison with experiments.
- The research has strong couplings with Navy experimental research programs, and provides theoretical support by predicting or designing new materials with specified properties.

RESEARCH AREAS

Computational Methods The Center supports the Office of Naval Research's Grand Challenge "Navy Materials by Design" by developing and maintaining a variety of computational tools. These include first-principles methods based on density-functional theory, specialized models for highly correlated systems, efficient tight-binding and overlapping-atom models, and simulation methods spanning multiple length scales.

Disordered Systems We study the nature of vibrons in disordered systems of various types using modeling and supercell methods. The characterization of normal modes in disordered crystals, glasses, amorphous materials, and materials with crystalline amorphous interfaces gives insight into thermal conduction and vibrational properties.



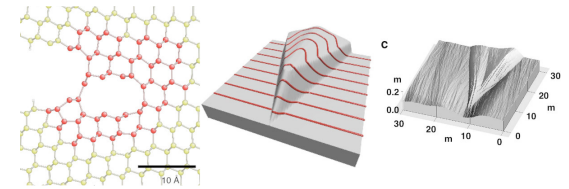
Gold catalyst particles on a tin-oxide substrate

Energy Storage and Generation This program is concerned with the modeling and prediction of materials that are efficient for storage or creation of energy. We use computational methods to understand the fundamental structural, electronic, and chemical processes that govern performance in Li-ion battery electrodes and fuel-cell catalysts and then apply those concepts to the design of new or improved materials.

Ferroelectrics We are using computational methods to understand the properties of these materials on an atomic level, and to identify avenues for improving existing materials and identifying new superior compositions.

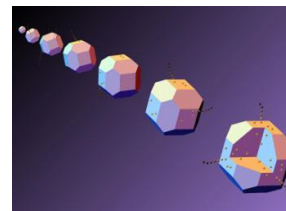
Magnetic Materials The Center studies a broad range of magnetic materials, from hard magnetic materials to dilute magnetic semiconductors. Some of these materials form the basis of current magnetoelectronic technologies, while others — both soft and hard magnets — are being studied for future applications. We are especially interested in low-dimensional and frustrated magnetism, as well as in the interplay between magnetism and superconductivity.

Mechanical Properties We apply computational methods including interatomic potentials, first principles, tight binding, and coupling of length scales approaches to the simulation of mechanical properties. Applications include static calculations of quantities such as ideal strength and ductility criteria, simulations of the evolution of microstructure, and multiscale simulations of dislocation properties and dynamic fracture.



Simulation of brittle fracture in silicon using coupling of length scales, showing crack-tip reconstruction, mesoscopic model, and experimental atomic-force microscope image of fracture surface.

Molecules and Clusters We predict how molecules and clusters respond when subjected to mechanical, electromagnetic, or chemical probes. Our interest is in exploiting properties which allow for information storage, environmental sensing, or energy conversion. This work is accomplished by predicting stabilities, reactivities, geometries, electronic and vibrational spectra, and magnetic properties.



Nanocrystals are doped during growth by adsorption of impurities on their exposed surface facets.

Nanostructures We investigate the properties of semiconductor nanostructures using both density-functional theory and semi-empirical methods. We are particularly interested in understanding and eventually controlling the process by which intentional impurities (dopants) are introduced into semiconductor nanocrystals. Currently we are developing new strategies, based on first-principles calculations, for choosing optimal dopants for specific semiconductor nanocrystals.

Quantum Computing A broad program is underway to use single-electron quantum dots in silicon for quantum information processing. A theoretical description of this system is necessarily multiscale, ranging from density functional theory at the atomic level to time-dependent model Hamiltonian calculations of many-dot systems. Optimal designs to minimize decoherence are being formulated.

Quantum Dots This research is focused on optical, magnetic, and transport properties of quantum dots, nanocrystals, and other nanostructures. New theoretical approaches are used to describe how these properties are modified by nanoscale confinement and to understand new physical effects that appear at this length scale.

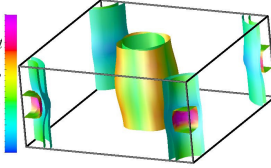
Electromagnetic Interactions in Matter Reduced-density-matrix approaches are developed for coherent electromagnetic interactions in quantized electronic systems, in the presence of environmental relaxation and decoherence phenomena. Particular interest is currently in electromagnetically induced transparency and related non-linear pump-probe optical phenomena in many-electron atomic systems and semiconductor quantum dots.

Superconductors The Center has been contributing to the understanding of novel superconductors since the discovery of high- T_c superconductivity in 1986. In recent years our main interest has been in the non-cuprate superconductors, including materials such as MgB_2 , the Ru-based superconductors, the fullerides, and, recently, the ferropnictides. We are interested in superconducting properties as well as both conventional (phonon-based) and unconventional (e.g. magnetic) mechanisms of superconductivity.

Surfaces and Interfaces We investigate the physics of clean and adsorbed surfaces of semiconductors and metals. Reduced dimensionality plays an important role at surfaces, profoundly influencing electronic and magnetic properties. We also study the interfaces between materials, which are at the heart of technologically important phenomena such as grain-boundary formation, band-offset engineering, and spin injection.

Thin Films We use density-functional calculations to optimize the growth and properties of thin films, primarily oxides. These films exhibit an enormous variety of phenomena, including metal-insulator transitions, superconductivity, ferroelectricity, piezoelectricity, and magnetism.

Fermi surface of a parent ferropnictide (LaFeAsO), colored according to the Fermi velocity.



POSTDOCTORAL PROGRAMS

Postdoctoral positions are available in the Center through the National Research Council and other programs. Annual stipends for postdocs in 2008 are approximately \$65000.

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