Computational Materials Sciences Awards

The Office of Basic Energy Sciences in the U.S. Department of Energy's Office of Science announced today three awards for research in Computational Materials Sciences in response to the solicitation DE-FOA-0001276. Awards total $8 million per year for four years starting in FY 2015. The research under these awards will integrate theory and computation with experiment and provide the materials community with advanced tools and techniques in support of the Materials Genome Initiative (MGI). MGI is an effort to reduce the time from discovery to deployment of new advanced materials by a factor of two with the goal to revitalize American manufacturing.

The lead institutions for the awards are Argonne National Laboratory, Brookhaven National Laboratory, and the University of Southern California. All will perform research that utilizes and develops community software for leadership class computing as well as for general use.

For this funding solicitation, integrated, multidisciplinary teams were sought to perform research and develop validated community codes and databases for predictive design of functional materials. Applicants proposed new approaches to enhance the use of large data sets derived from advanced characterization of materials, materials synthesis, processing, properties assessments, and the data generated by large-scale computational efforts that model materials phenomena. Awards were selected from a large number of applications following rigorous peer review of their scientific and technical merit, proposed budget, competency of the team, and management plan.

The projects are expected to develop open-source, robust, validated, user-friendly software (and the associated experimental and computational databases) that captures the essential physics and chemistry of relevant systems and can be used by the broader research community and by industry to accelerate the design of new functional materials. The goal of this research activity is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software, coupled with innovative use of experimental and theoretical data, enables the design, discovery, and development of new materials, and in turn, creates new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences is a critical area in which the United States needs to be competitive in the 21st century through global leadership in innovation.

Project Descriptions:

Midwest Integrated Center for Computational Materials

Team: Principal Investigator, Giulia Galli, Argonne National Laboratory. Partners: University of Chicago, University of Michigan, Northwestern University, University of Notre Dame, and University of California-Davis.

Goals: Development of interoperable quantum, classical and particle-continuum software, enabling the simulation and prediction of functional materials for energy conversion processes, with an emphasis on interfaces, the transport across them, and the manipulation of matter under conditions far from equilibrium. Validation of materials specific predictions includes

experiments at the Advanced Photon Source and the Center for Nanoscale Materials. Data management and computing will primarily use capabilities at the Argonne Leadership Computing Facility.

Center for Computational Design of Functional Strongly Correlated Materials & Theoretical Spectroscopy

Team: Principal Investigator, Gabriel Kotliar, Brookhaven National Laboratory. Partners: Rutgers University, University of Tennessee, and Ames Laboratory.

Goals: Development of next-generation methods and software to accurately describe electronic correlations in oxides and complex materials and a companion database to predict targeted properties with energy-related application to thermoelectric materials. Validation of materials specific predictions includes experiments at the National Synchrotron Light Source II. The project will use capabilities at the National Energy Research Scientific Computing Center (NERSC), and the Argonne and Oak Ridge Leadership Computing Facilities.

Computational Synthesis of Materials Software Project with Validation on Layered Low Dimensional Functional Materials and Ultra-Fast X-Ray Laser Experiments

Team: Principal Investigator, Priya Vashishta, University of Southern California. Partners: California Institute of Technology, Lawrence Berkeley National Laboratory, University of Missouri, Rice University, and SLAC National Accelerator Laboratory.

Goals: Development of next-generation methods and software to predict and control materials processes at the level of electrons for synthesis, intercalation and exfoliation of stacked, two-dimensional, functional layered materials with energy-related application to electronics and catalysis. Validation of materials specific predictions includes ultrafast free electron laser experiments at the Linac Coherent Light Source. Data management integrates the Materials Project at Lawrence Berkeley National Laboratory and uses computing capabilities at NERSC and the Argonne Leadership Computing Facility.