

Computational Research in Heterogeneous Catalysis

Center for Nanophase Materials Sciences Oak Ridge National Laboratory Oak Ridge, Tennessee

ORNL07-75-CNMS

Project Description:

The Catalysis and Nano-Building Blocks group of the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) is seeking a post-doctoral research associate to conduct computational research on heterogeneous catalysis. In recent years electronic structure-based theoretical methods, especially density functional theory (DFT), have seen substantial development and increasing acceptance as a valuable tool for advancing nanoscience, including catalysis. DFT has been successfully applied to unravel reaction mechanisms at the molecular level and design new catalytic materials with tailored properties. It is expected that the candidate will use DFT calculations, coupled with other computational methods (reaction pathway search, kinetic Monte Carlo, etc.) to investigate and elucidate the reactivity of small organic molecules on transition metals.

The candidate will work in close collaboration with computational staff at the CNMS to develop concrete strategies to modify and improve existing catalyst formulations of specific interest to the program sponsors. The CNMS, one of the five DOE nanoscience research centers, offers a highly collaborative atmosphere and world-class computational facilities. Diverse theoretical and computational expertise is coupled closely to experimental research at the Center. This project will be funded in part by a contract with Eastman Chemical Company. Although a portion of the work will be proprietary, it is expected that the candidate will publish non-proprietary research results in the open literature.

Qualifications: The successful candidate must have a Ph.D. in chemistry, chemical physics, chemical engineering, or material science and must have substantial experience with atomistic simulation. Proven background in catalysis and the use of density functional theory (DFT) to probe molecular transformations, in particular with relation to surface chemical reactions, is expected. Strong communication skills, including demonstrable ability to communicate effectively with experimentalists, and good judgment and accountability are required. Applicants cannot have received the most recent degree more than five years prior to the date of application and must complete all degree requirements before starting their appointment.

How to Apply:

Qualified applicants may apply online at https://www2.ornl.gov/ORNL_POST/. All applicants will need to register before they can begin the online application. For complete instructions, on how to apply, please see the instructions at <http://www.ornl.gov/orise/edu/ornl/ornl-pdpm/application.htm>. **When applying for this position, please reference the position title and number (ORNL07-75-CNMS).**

This appointment is offered through the ORNL Postdoctoral Research Associates Program and is administered by Oak Ridge Associated Universities (ORAU). This appointment is open to all qualified U.S. and non-U.S. citizens without regard to race, color, age, religion, sex, national origin, physical or mental disability, or status as a Vietnam-era veteran or disabled veteran.