



## **Postdoctoral Research Associate Position**

### **Computational Nanocatalysis**

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

**ORNL11-64-CNMS**

The Chemical Functionality Group of the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) is seeking a postdoctoral research associate to conduct computational research in nanocatalysis. In recent years electronic structure-based theoretical methods, especially density functional theory (DFT), have seen substantial development and widespread acceptance as a valuable tool for advancing the science of catalysis. In particular theory has been successfully applied to design new catalytic materials with tailored properties. The candidate will work in close collaboration with our computational staff and use DFT coupled with other modeling techniques to investigate the properties and reactivity of supported small metal clusters. It is expected that this research will lead to the development of novel cluster-based catalytic materials for important energy-related catalytic processes. The [CNMS](#) is a collaborative nanoscience user research facility established by the Office of Science, U.S. Department of Energy. Diverse theoretical and computational expertise is coupled closely to experimental research at the Center.

#### **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 using first-principles methods to probe molecular transformations, in particular surface chemical reactions, and programming experience are required. Strong communication skills, including demonstrable ability to communicate effectively with experimentalists, and good judgment and accountability are also required. Applicants must have received their highest degree not more than five years prior to the date of application and must complete all degree requirements before starting their appointment.

#### **Technical Questions**

For more information about this position please contact Dr. Ye Xu ([xuy2@ornl.gov](mailto:xuy2@ornl.gov)) and reference this position title and number in your correspondence. Applications will be accepted until the position is filled.

#### **How to Apply**

Qualified applicants may apply online at [https://www2.ornl.gov/ORNL\\_POST/](https://www2.ornl.gov/ORNL_POST/). All applicants will need to register before they can begin the online application. For complete information on how to apply please see the instructions at <http://www.ornl.gov/orise/edu/ornl/ornl-pdpm/application.htm>.

This appointment is offered through the ORNL Postgraduate Research Participation Program and is administered by the Oak Ridge Institute for Science and Education (ORISE). 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.