

# ORNL Publications

## External Publication

### Job Posting Title

Research & Development Staff Member / NB50483895

### Posted Date

06/09/2015

### End Posting Date

07/08/2015

### Purpose

The Chemical Sciences Division, Physical Sciences Directorate at Oak Ridge National Laboratory (ORNL) is seeking an early career Computational Chemist to focus on modeling the interplay of chemical reactions at fluid-solid interfaces and transport in porous media in chemical, materials and geologic sciences. Due to the inherently multi-scale nature of these processes, the successful candidate should be comfortable addressing processes at atomic to macroscopic scales. In particular the candidate should have expertise in computational modeling, simulations and code development pertaining to the hydrodynamic flow regime. The candidate will benefit from the diverse fundamental research program in the Chemical Sciences Division and the unique capabilities at ORNL including world class computing (National Center for Computational Science), Spallation Neutron Source and High Flux Isotope Reactor, and Center for Nanophase Materials Sciences.

### Major Duties/Responsibilities

- Model the interplay of chemical reactions at fluid-solid interfaces and transport in porous media
- Work independently and with experimentalists to develop validated, predictive models that move beyond the current length and time scale limitations
- Publish results in high-quality, peer-reviewed journals in a timely manner and make presentations at professional and all-hands meetings
- Contribute to peer-reviewed proposal development utilizing new computational methods to understand mesoscale processes and participate in major initiatives across the laboratory
- Ensure compliance with environment, safety, health and quality program requirements
- Maintain strong commitment to the implementation and perpetuation of values and ethics

### Qualifications Required

- PhD in Physical Sciences, Mathematics, Computational Science or a closely related field with at least 2 years of experience
- Experience in the application of computational approaches in chemical, geochemical, materials science or physics
- Expertise in computational modeling, simulations and code development pertaining to the hydrodynamic flow regime
- Expertise in modeling realistic chemical reactions, such as sorption, precipitation/dissolution and heterogeneous catalysis
- Experience in high performance computing
- Flexibility and understanding of experimental and computational methods and theories
- Excellent interpersonal skills, and ability to communicate in English orally and in writing to a scientific audience
- Strong record of productive and creative research, demonstrated by publications in peer-reviewed journals and presentations at scientific conferences
- Capability of working collaboratively in a team environment and interacting effectively with a broad range of colleagues

across both national and international institutions

Desired Qualifications:

- Expertise in simulation methods include, but are not limited to, Navier-Stokes, Smoothed Particle Hydrodynamic methods, coarse-grained atomistic simulation, and kinetic Monte Carlo.

### ***Work Directions and Interfaces***

Position reports to the Group Leader, Geochemistry & Interfacial Sciences Group in the Chemical Sciences Division. Interfaces with administrative staff, managers and visitors to ORNL.

This position will remain open for a minimum of 5 days after which it will close when a qualified candidate is identified and/or hired.

We accept Word(.doc, .docx), Excel(.xls, .xlsx), PowerPoint(.ppt, .pptx), Adobe(.pdf), Rich Text Format(.rtf), HTML(.htm, .html) and text files(.txt) up to 2MB in size. Resumes from third party vendors will not be accepted; these resumes will be deleted and the candidates submitted will not be considered for employment.

If you have trouble applying for a position, please email [ORNLRecruiting@ornl.gov](mailto:ORNLRecruiting@ornl.gov).

Notice: If the position requires a Security Clearance, reviews and tests for the absence of any illegal drug as defined in 10 CFR 707.4 will be conducted by the employer and a background investigation by the Federal government may be required to obtain an access authorization prior to employment and subsequent reinvestigations may be required.

If the position is covered by the Counterintelligence Evaluation Program regulations at 10 CFR 709, a counterintelligence evaluation may include a counterintelligence-scope polygraph examination.

ORNL is an equal opportunity employer. All qualified applicants, including individuals with disabilities and protected veterans, are encouraged to apply. UT-Battelle is an E-Verify Employer.