

# ORNL Publications

## External Publication

### Job Posting Title

Postdoctoral Research Associate –Theory and Modeling of Beam (Electron, Ion)-Matter Interactions / NB50648197

### Posted Date

12/13/2017

### End Posting Date

01/13/2018

### Purpose

We are looking for a Postdoctoral Research Associate to work on developing an understanding of energy transfer at a quantum mechanical level, from focused electron and ion beams to matter at the nanoscale (solid, liquid, gas). In this role you will closely collaborate with a diverse group of experimentalists, theorists, and data scientists as part of the Center for Nanophase Materials Science (CNMS) in-house science as well as work with staff and capabilities in high performance computing. This is a joint position between the Nanomaterials Theory Institute and Scanning Probe Microscopy Group within the CNMS of the Physical Sciences Directorate (PSD) at the Oak Ridge National Laboratory (ORNL).

### OVERVIEW:

The mechanisms that govern how energy is imparted from a highly focused beam of energetic electrons or ions to materials are not always well understood or captured by existing theory, models, or simulations. This is especially true in cases when the system in question is highly confined, such as a single molecule on a surface or a defect or interface within a material, which are conditions of particular interest to our work at the CNMS that is focused on Directed Nanoscale Transformations.

As a postdoc, your research will focus on developing the underlying theoretical descriptions, accurate models and simulations approaches necessary to understand and predict nanoscale transformations caused from beam (electrons, ions) matter (solid, liquid, gas) interactions such as energy transfer processes and cascading reactions. In particular, understanding the effects of confinement on locally driven chemical reactions, and conversely, how reaction processes and pathways affect the selection and confinement of reaction products. The research will be directly integrated with ongoing experimental work with the overall goal of directing matter with atomic precision to create 3D nanoscale structures that have desired form and function.

### Major Duties/Responsibilities

#### IN THIS POSITION YOU WILL:

- Work as part of a dynamic team conducting CNMS in-house research that advances our understanding of nanomaterials while also leading to the development of capabilities that will eventually become available to the CNMS user community
- Develop & apply computational, first principles models of interaction of ions/electrons/external field with materials based on density functional theory (DFT)/approximate DFT and time-dependent quantum mechanics
- Perform data analysis and interpretation
- Present research and publish scientific results in peer-reviewed journals in a timely fashion
- Work with others to maintain a high level of scientific productivity
- Ensure compliance with environment, safety, health, and quality program requirements

- Maintain strong dedication to the implementation and perpetuation of values and ethics

### **Qualifications Required**

Basic Qualifications - To be considered for this position, you must have:

- A Ph.D. in physics, materials science and engineering, chemistry, or a closely related discipline completed within the last five years
- Strong programming skills with Fortran and/or C/C++
- Experience with Unix/Linux
- Experience with at least one of the following high-level programming languages: Python, Matlab, Octave
- Experience with the application and development of electronic structure calculations

Preferred Qualifications – This experience is to your advantage:

- Background programming with any electronic structure package
- Experience with MPI, GPU programming and DFTB
- Relativistic quantum chemistry
- Experience using Jupyter notebooks
- A strong record of productive and creative research demonstrated by publications in peer-reviewed journals and presentations at scientific conferences
- Excellent written and oral communication skills and the ability to communicate in English to an international scientific audience
- Capability for innovative research with minimal supervision and the ability to work collaboratively in a team environment and interact effectively with a broad range of colleagues
- Ability to work well in a dynamic research environment, set priorities to accomplish multiple tasks within deadlines, and adapt to ever-changing needs

### **OTHER INFORMATION:**

Applicants cannot have received their Ph.D. more than five years prior to the date of application and must complete all degree requirements before starting their appointment. The appointment length will be up to 24 months with the potential for extension. Initial appointments and extensions are subject to performance and availability of funding.

Please provide a list of publications when applying for this position. Three letters of reference are required and can be uploaded to your profile or emailed directly to [PSDrecruit@ornl.gov](mailto:PSDrecruit@ornl.gov). Please include the title of the position in the subject line.

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.