

TITLE: Atomistic and multiscale machine learning for predictive semiconductor heterointerface design (U.S. Citizens preferred)

#### Overview

The Materials Measurement Laboratory of the National Institute of Standards and Technology is seeking qualified persons (U.S. Citizens preferred) to develop advanced atomistic machine learning (ML) capabilities with applications in multiscale predictive semiconductor heterointerface and device design. The candidate will contribute to algorithm design for accelerated atomistic simulation of device fabrication processes and defect formation and ML-based property prediction.

#### Duties

- Develop and apply novel reinforcement learning methods for accelerated prediction of heterointerface structure and defect energetics, with particular focus on semiconductor devices
- Develop and apply multiscale machine learning methods for predictive modeling and design of semiconductor devices, bridging models at the material property and continuum device level.
- Collaborate with team members to train and evaluate scalable and chemically transferrable ML force fields to support the above multiscale modeling responsibilities, as well as to develop reference, validation, and training datasets, and to deploy ML for rapid screening and property calculations.
- Perform computational experiments in a reproducible and well documented manner.
- Ensure archival publication of results, protocols, software, and documentation.

#### Required Skills, Expertise and Qualifications

- Ph.D. in Materials Science, Physics, Chemistry, or a related field.
- Strong communication skills: multiple lead author publications and conference presentations on applied machine learning for materials simulation and characterization.
- Demonstrated experience developing reinforcement learning approaches for material simulation. Strong preference for experience with continuous action spaces for atomistic systems.
- Demonstrated experience with uncertainty quantification and dataset bias evaluation.
- Strong experience with atomistic modeling of multiphase materials and interfaces: experience performing density functional theory calculations, molecular dynamics, and Monte Carlo.
- Ability to work with atomistic simulation data at scale.
- Strong experience in multiple programming languages (Python, C/C++, Julia, etc.) and familiarity with parallel computing technologies (such as MPI and CUDA).
- Excellent communication and teamwork skills for interdisciplinary collaboration.

Employment Terms: This opportunity is to be an associate researcher in the NIST Materials Measurement Science Division for a term of one year, with options to renew. Associate researchers are NOT federal employees, but they work alongside NIST researchers and with NIST's often world-class instrumentation. Relocation expenses will not be provided. U.S. Citizens hired into associate positions may have the opportunity to seek longer term Federal Employment.

Salary: up to \$89,000 annually, commensurate with the candidate's qualifications and experience

How to express interest: Persons (US Citizens preferred) who meet all of the required qualifications and who would be interested in taking this position are invited to express their interest by sending an email that briefly describes their qualifications along with a CV to [643assoc@nist.gov](mailto:643assoc@nist.gov). US Citizens should note "US Citizen" and the opportunity title in the email subject line. All others should note "Non-US Citizen" and the opportunity title in the email subject line.