

NIST/MML/MSED Research Associate Opportunity

TITLE: Developing High-Throughput Density Functional Theory Workflows for Material Property Prediction

Overview

The Materials Measurement Laboratory of the National Institute of Standards and Technology is seeking qualified persons (U.S. Citizens preferred) to develop a multi-scale modeling infrastructure for the predicting the properties and performance of advanced semiconductor materials and devices. This position will focus on developing high throughput density functional theory (DFT) workflows to accelerate material property prediction of semiconductor of materials. Some of the key properties to be predicted include the electronic structure, bandgaps, band alignments and transport properties, and defects.

Duties

- Development of a streamlined workflow to conduct high-throughput calculations for semiconductor-specific properties.
- Calculate properties such as bandgaps, band offsets, Schottky barriers, current-voltage curves, mobility, and thermal conductivity.
- Presenting results at internal meetings, and occasional meetings with external stakeholders.

Required Skills, Expertise and Qualifications

- Ph.D. in Materials Science and Engineering or a related field.
- Experience with using various first-principles simulation codes such as, VASP, Abinit or QuantumATK.
- Experience with using Scikit-Learn to perform machine learning surrogate model development
- Python expertise.
- Excellent written and oral communication skills.

Employment Terms: This opportunity is to be an associate researcher in the NIST Materials Science and Engineering Division for a term of 1 year, with options to renew. Associate researchers are NOT Federal Employees, but they work along with 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: Between \$82,000 and \$87,000, based on qualifications and experience.

How to express interest: Interested persons (U.S. Citizens preferred) who meet all of the required qualifications are invited to express their interest by sending an email that briefly describes their qualifications along with a CV to 642assoc@nist.gov. U.S. 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.