NIST/MML/MSED Research Associate Opportunity

TITLE: Developing Atomistic Transport Calculations for Semiconductor Materials

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 via atomistic simulations to obtain transport properties via non-equilibrium Green's function (NEGF) techniques. Some of the key properties include conductance, I-V characteristics and transmission spectra. A key aspect of this work will be exploring how defects impact the transport properties of industrially relevant semiconductor interfaces. The systems of interest include gate-all-around transistors (Si/SiO_2), high power devices (SiC/SiO_2) and high electron mobility transistors (GaN/AlGaN).

Duties

- Develop comprehensive workflow to conduct high-throughput NEGF calculations to obtain conductance, I-V characteristics and transmission spectra for semiconductor interfaces.
- Perform simulations using atomistic (electronic structure and transport) software such as VASP, Quantum Espresso, GPAW, DFTB+, SIESTA/TranSiesta, QuantumATK, or similar codes, and perform data analysis, to investigate relevant material properties.
- Use NEGF in conjunction with machine learning techniques to study electronic transport phenomena at a larger scale.
- 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 DFT and atomistic transport software: VASP, Quantum Espresso, GPAW, DFTB+, SIESTA/TranSiesta, QuantumATK.
- Python programming, and experience with machine learning techniques.
- Excellent written and oral communication skills are required for collaboration and should be evident in archival publications.

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.