

TITLE: Postdoctoral Researcher Applying Machine Learning Methodologies to Predict Spectra of PFAS Compounds (U.S. Citizens preferred)

Overview

The Material Measurement Laboratory of the National Institute of Standards and Technology is seeking qualified persons (U.S. Citizens preferred) to apply modern methods in artificial intelligence (AI) and machine learning (ML) to the problem of predicting infrared spectra and mass spectra for PFAS compounds. The candidate should have a strong background in AI/ML with application to chemical problems, have familiarity with infrared and mass spectra, and understand the relevant chemistry of PFAS molecules. This position will involve working with a team of chemists, physicists, mathematicians, data scientists and machine learning experts characterizing PFAS molecules used in the semiconductor industry with the goal of discovering new molecules for the semiconductor etching process.

Duties

- Develop libraries of training data through mining of existing databases and simulation of infrared and mass spectra using quantum chemistry and related methodologies.
- Create AI/ML models for high-fidelity prediction of the infrared and mass spectra and validate their use in matching experimentally-measured spectra.
- Collaborate with other computational and experimental researchers to meet project goals.
- Disseminate results through publications, talks, poster presentations, etc.

Required Skills, Expertise and Qualifications

- Ph.D. in chemistry, physics, or a closely aligned field.
- Demonstrated experience in conducting quantum scattering calculations.
- Strong programming skills in languages such as Python or C/C++, experience using modern software frameworks for AI/ML, and experience in data analysis.
- Motivated, independent researcher with good organizational, communication and leadership skills.
- Solid track-record of scientific publication.

Employment Terms: This opportunity is to be an associate researcher in the NIST Chemical Sciences 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: \$90k – \$110k, commensurate with experience.

How to express interest: Persons (U.S. 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 646assoc@nist.gov. U.S. Citizens should note "U.S. Citizen" and the opportunity title in the email subject line. All others should note "Non-U.S. Citizen" and the opportunity title in the email subject line.