

**PREP Research Associate
CHIPS Funded Project**

This position is part of the National Institute of Standards and Technology (NIST) Professional Research Experience Program (PREP). NIST recognizes that its research staff may want to collaborate with researchers at academic institutions on specific projects of mutual interest and, therefore, requires those institutions to be recipients of a PREP award. The PREP program involves staff from a wide range of backgrounds conducting scientific research across various fields. Individuals in this position will perform technical work supporting the collaboration's scientific research.

Research Title:

Postdoctoral Researcher Applying Machine Learning Methodologies to Predict Spectra of PFAS Compounds

The work will entail:

The Materials 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.

U.S. Citizen Preferred

Key responsibilities will include but are not limited to:

- 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.

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.

Privacy Act Statement

Authority: 15 U.S.C. § 278g-1(e)(1) and (e)(3) and 15 U.S.C. § 272(b) and (c)

Purpose: The National Institute for Standards and Technology (NIST) hosts the [Professional Research Experience Program \(PREP\)](#) which is designed to provide valuable laboratory experience and financial assistance to undergraduates, post-bachelor's degree holders, graduate students, master's degree holders, postdocs, and faculty.

PREP is a 5-year cooperative agreement between NIST laboratories and participating PREP Universities to establish a collaborative research relationship between NIST and U.S. institutions of higher education in the following disciplines including (but may not be limited to) biochemistry, biological sciences, chemistry, computer science, engineering, electronics, materials science, mathematics, nanoscale science, neutron science, physical science, physics, and statistics. This collection of information is needed to facilitate the administrative functions of the PREP Program.

Routine Uses: NIST will use the information collected to perform the requisite reviews of the applications to determine eligibility, and to meet programmatic requirements. Disclosure of this information is also subject to all the published routine uses as identified in the Privacy Act System of Records Notices: NIST-1: NIST Associates.

Disclosure: Furnishing this information is voluntary. When you submit the form, you are indicating your voluntary consent for NIST to use of the information you submit for the purpose stated. By applying to a CHIPS-funded PREP opportunity, you also acknowledge that participation in the project requires signing a Non-Disclosure Agreement (NDA) prior to beginning any work.