

**PREP Research Associate
CHIPS Funded Project**

This position is part of the National Institute of Standards (NIST) Professional Research Experience (PREP) program. NIST recognizes that its research staff may wish to collaborate with researchers at academic institutions on specific projects of mutual interest and thus requires that such institutions be the recipients of a PREP award. The PREP program requires staff from a wide range of backgrounds to work on scientific research in many areas. Employees in this position will perform technical work that underpins the scientific research of the collaboration.

Research Title:

Quantum Scattering Calculations of Rates and Ion-Molecule Cross Sections of PFAS Compounds

U.S. Citizen Preferred

The work will entail:

- Perform quantum scattering calculations of small PFAS molecules as well as possible replacement compounds for use in plasma etching of semiconductor chips using a suitable code (e.g. UKRMol+).
- Extending the capability of a scattering code to enable project goals.
- Collaborate with other project members to predict ion-molecule cross sections and reaction rates using machine learning models.
- Compare calculated results to results from other calculations and from experiment.
- Potentially interface with CFD modelers to incorporate calculated data into their models.
- Work to develop a knowledge base of the important properties of PFAS molecules for the etch process as a means of guiding the search for replacement compounds.
- Develop software to implement the goals stated above using an appropriate computer language (e.g., Fortran, C/C++, Python).
- Disseminating results through posters/seminars at international meetings and university seminars.
- Ensuring that all results, findings, data, software, etc. are correctly archived and transmitted through appropriate channels.

Key responsibilities will include but are not limited to:

- Algorithm development, implementation and analysis.
- Scientific and technical programming.
- Computation and analysis of data.
- Presentation of results at internal meetings, and occasional meetings with external stakeholders.

- Publication of results in appropriate journals and publication of data to a web-based database.
- Ensure that results, protocols, software, and documentation have been archived or otherwise transmitted to the larger organization.

Qualifications

- A Ph.D. degree in Chemistry, Physics, Mathematics, Computer Science, Data Science, or a related field.
- 4+ years of relevant experience. Experience in quantum scattering calculations is required.
- Significant course work in one or more of chemistry, physics, mathematics, statistics and/or computer science.
- Ability to program in a modern computational language (e.g., Fortran, C/C++, Python).
- Strong oral and written communication skills.

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.