

TITLE: Postdoctoral Researcher Calculating Scattering Cross Sections and Reaction Rates of PFAS Molecules (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 conduct quantum mechanical scattering calculations of ion-molecule cross sections and reaction rates using a suitable scattering code (e.g. UKRMol+, Astra). The candidate will study PFAS molecules currently used in semiconductor etching processes and contribute to a collection of high-fidelity data targeted for use in plasma modeling. This position will involve working with an interdisciplinary team of chemists, physicists, mathematicians, data scientists and machine learning experts to characterize PFAS molecules used in the semiconductor industry with the goal of discovering new molecules for the etching process.

Duties

- Conduct calculations of ion-molecule cross sections and reaction rates of PFAS molecules using modern molecular scattering codes
- Conduct high-level quantum chemistry calculations of the target molecules to provide input to the scattering calculations
- 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 C/C++, Fortran, Python 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.