PREP Research Associate

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, thus requires that such institutions must be the recipient 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:
Interpretable DNA/RNA Ensemble Quantification (Molecular dynamics, machine learning, measurement analysis)

The work will entail:
This position will focus on theory and computation to classify DNA and RNA conformational ensembles using secondary-structure-based distance metrics and clustering. A central goal is to build hierarchical, interpretable ensemble representations that connect simulation-derived clusters to experimental measurements/observables and statistical-physics interpretation (e.g., energetic barriers and kinetic pathways). Work includes developing and validating analysis algorithms, implementing reproducible research software, and collaborating with experimental and device-focused teams to connect theory outputs to measurement needs.

Key responsibilities will include but are not limited to:

- Develop, test, and extend ensemble representations for DNA/RNA and relate these to experimental observables,
- Implement and optimize secondary-structure distance metrics based on base-pair reorganization,
- Build scalable clustering and model-selection for large molecular dynamics datasets,
- Presenting results at internal and external meetings and conferences,
- Develop well-documented, reproducible research software and publish results.

U.S. Citizen Preferred

<u>Qualifications</u>

- A Ph.D. in physics, chemistry, biophysics, computational biology, applied mathematics, computer science, or a closely related field.
- Demonstrated experience with biomolecular simulation and/or trajectory analysis (strong preference for nucleic acids: DNA/RNA).
- Experience with coarse-grained nucleic-acid models, e.g., oxDNA/oxRNA or closely related coarse-grained frameworks.
- Practical understanding of clustering/unsupervised learning and distance-metric design.

- Strong scientific programming (Python preferred; Julia a plus) and ability to write maintainable, version-controlled code.
- Background in statistics/statistical physics; ability to interpret ensembles in terms of kinetics and free-energy landscapes.
- Strong written and oral communication skills and ability to collaborate in a multidisciplinary team; experience analyzing experimental data from single-molecule and ensemble techniques is a plus.

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 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.