Computational Investigation of the Structure, Dynamics, and Design of Ice-Nucleating Proteins

About AFRL:

The biomaterials group under the materials research directorate at the Air Force Research Lab (AFRL) participates in the High-Performance Computing Internship Program (HIP) offered by the Department of Defense High Performance Computing Modernization Program (DoD-HPCMP). The biomaterials group has been mentoring students from the science and engineering fields since 2008 (under JEOM and HIP) and seeks students for internship opportunities where they receive training in state-of-the-art high-performance computing on projects relevant to the DoD mission and/or their future careers.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

Ice-nucleating proteins (INPs) are a family of proteins that promote the nucleation of ice at higher temperatures. As average global temperatures rise, the permafrost upon which Arctic DoD installations are built begins to melt. Therefore, a solution for keeping the permafrost frozen at higher ambient temperatures has become increasingly necessary. One such solution can be found in INPs. As part of a strong collaboration with our experimental colleagues, the modeling team at AFRL/RXEB will mentor a FIX faculty member to research in the computational investigation of INPros as a means of stabilizing DoD installations in cold regions.

The scientific problems addressed by this project are two-fold: 1) investigate the mechanism that underlies the ability of ice nucleating proteins (INPros) to efficiently nucleate ice, and 2) identify and/or design candidate INPros for further experimental investigation. Solving these problems will require a variety of computational techniques, including, but not limited to de novo protein structural modeling, molecular dynamics simulations, bioinformatics (including static and dynamic network analysis of protein-protein, residue-residue, water-water, and water-protein interaction networks), and machine learning using network data.

As part of achieving its mission to support DoD interests, the AFRL BioRT modeling group has historically made significant use of DoD HPC resources. For this project, significant computational hours on DoD supercomputers will be required to perform and analyze molecular dynamics simulations characterizing INPros that the group has modeled using de novo protein structure prediction tools (AlphaFold3). Hours will also be used to train machine learning models to predict properties related to ice nucleation efficiency.

The faculty member will collaborate closely with scientists, interns, and other faculty within the BioRT modeling group to conduct novel research using HPC resources, all while gaining experience within and outside of their field of expertise. While day-to-day activities of a faculty member depend strongly on the nature of the project initiated, typical activities from previous years are listed below:

1.) Training: The faculty member will attend training workshops provided by AFRL/AFIT and gain experience working with the "tools of the trade" in modeling and simulation.

- The faculty member can participate in tours of local HPC facilities to gain an understanding of the operational support of the HPC systems they use.
- Faculty members are encouraged to use local courses to expand their knowledge of the breadth and depth of HPC applications available to them for conducting their research.

2.) Professional Networking and Data Dissemination: Examples of previous and expected routes of data dissemination and networking:

- The faculty member will participate in local meetings, presenting findings at computational group meetings, research team meetings, and branch-wide research meetings. Additionally, the DoD-HPCMP holds an end-of-summer HIP/FIX research symposium where the faculty member will share their findings and experience in an oral presentation.
- Faculty members are encouraged to disseminate findings in poster sessions and oral presentations at regional and national conferences.

ANTICIPATED START DATE:

May 2025 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

The ideal candidate must be full-time faculty member from an accredited U.S. pre-college, college, or university in a science or engineering field with a background in modeling and simulation. In particular, experience with any of the following is highly valued:

- Classical molecular dynamics codes (e.g., NAMD, GROMACS, LAMMPS, OpenMM, or CHARMM)
- Ab initio methods (e.g., DFT)
- Machine learning and data science techniques
- Bioinformatics/molecular biology and its sub-fields (e.g., interactomics) and methods (e.g., sequence/structure alignment)
- High performance, parallel software development methods (e.g., MPI, CUDA)

Adjunct or visiting faculty are ineligible.

ACADEMIC LEVEL:

- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Science
- Computer, Information, and Data Sciences
- Engineering
- Physics
- Science and Engineering related