

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-FIX-24-021-F

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 INPs as a means of stabilizing DoD installations in "cold regions."

The scientific problems addressed by this project are two-fold: 1) investigate the mechanism of action of ice nucleating proteins (INPs), particularly their effect on the point of liquid-liquid phase separation (LLPS) and 2) identify candidate INPs 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, and bioinformatics (including static and dynamic network analysis of protein-protein and residue-residue interaction networks).

As part of achieving its mission to support DoD interests, the AFRL BioRT modeling group has historically made significant use of DoD HPC resources, and it will continue to do so for the duration of this project. Significant computational hours on DoD supercomputers will be required to perform molecular dynamics simulations to characterize systems containing a collection of INPs that the group will model using de novo protein structure prediction tools (AlphaFold2).

ANTICIPATED START DATE:

May 2024 – 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 limited background in data handling and program operation typical to HPC. This internship will help the faculty member improve their capability to formulate pertinent scientific questions and use HPC to answer them. Adjunct or visiting faculty are ineligible.

ACADEMIC LEVEL:

- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Science
- Computer, Information, and Data Sciences
- Engineering
- Life Health and Medical Sciences
- Mathematics and Statistics
- Physics
- Science and Engineering related