

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-022

Understanding Bio sequestration of Rare Earth Elements through Protein Modeling using the DoD-HPC

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:

The proposed plan includes two major components that will need to be accomplished in the presented order: optimization of the REE force field parameters to reproduce experimentally observed osmotic coefficients and dissociation constants; and running molecular dynamics simulations to measure the binding affinity through free energy perturbation (FEP) and umbrella sampling methods. The HIP intern should be familiar in Python and R for the major coding components of the analysis. Bayesian optimization is performed in Python, so familiarity with statistical optimization techniques in Python would also be desirable. The intern will also perform molecular dynamics simulations using different engines such as GROMACS and NAMD. We aim to generate an automated software suite for REE force field generation based upon experimental data (structural and energetic). This suite can be used in the future to develop and validate improved force fields as more experimental data becomes available. This modular workflow can be used for multiple projects to develop force fields in a timely and efficient manner on the DoD-HPC.

Each summer, scores of interns are present in the Materials and Manufacturing Directorate (AFRL/RX) laboratories. While day-to-day activities of an HPC intern depend strongly on the nature of the project initiated, typical activities from previous years are listed below:

1.) Training:

The student will attend training workshops provided by AFRL/AFIT and surrounding institutions, such as resume and publication writing workshops, and will be encouraged to develop presentation skills via poster or oral presentations.

2.) Professional Networking and Data Dissemination:

Examples of previous and expected routes of data dissemination and networking:

- Student will participate in local meetings, presenting findings at computational group meetings, research team meetings, and branch-wide research meetings. Also, AFRL/RX holds a student poster session at the end of each summer.

- Student is encouraged to disseminate findings in poster sessions and oral presentations at regional and national conferences. Previously, students in this group have presented findings at regional conferences of the ACS Regional meeting, the National Graduate Polymer Research Conference, the ASM International regional meeting, the ACS National Meeting and Exposition and APS Meetings.
- It is expected the student will participate in tours of local HPC facilities to gain an understanding of the operational support of the HPC systems they use.
- Students are encouraged to use local courses to expand their knowledge of the science behind the simulations as well as the breadth and depth of available HPC applications.

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 will be a student in a science or engineering field with limited background in data handling and program operation typical to HPC. This internship will help the student improve their capability to formulate pertinent scientific questions and use HPC to answer them.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- 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