

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-FIX-24-022-F

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:

Reliable extraction and separation of Rare Earth Elements (REEs) from feedstock is a notoriously challenging process due to similar chemical properties (such as ionic radius) across the lanthanide series. Existing extraction processes rely on environmentally harmful solvents. This project utilizes computational modeling to assist the development of an environmentally friendly extraction process using REE-binding proteins.

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 FIX faculty member 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. Under the guidance of a mentor, the faculty member will also perform molecular dynamics simulations using different engines such as GROMACS and NAMD. The goal is 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.

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