

**Opportunity Title:** High Performance Computing Internship Program: Air Force Research Laboratory  
**Opportunity Reference Code:** ERDC-ITL-2023-0012

**Organization** U.S. Department of Defense (DOD)

**Reference Code** ERDC-ITL-2023-0012

**How to Apply** Click on *Apply* now to start your application.

**Description** 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). AFRL 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 Air Force needs and/or their future careers.

Numerous proteins of interest to support DoD mission such as lanmodulin (LanM) for bio-extraction of rare earth elements (REEs), antifreeze proteins (Arctic Strategy), and dehalogenases for removing per- and poly-fluoroalkyl substances (PFAS). For the analysis of protein structures, the residue-interaction network (RIN) analysis is an effective approach to understand how the proteins interact with the ligands (REEs, ice, PFAS substrates, etc.) and how protein dynamics drives their function. Developing effective codes and workflows to perform RIN analysis on the DoD-HPC supercomputers is required for accelerating these DoD missions.

#### What will I be doing?

Under the guidance of the mentor, you will perform de novo structure modeling and MD simulations. The key problems addressed include: constructing the distance matrices from the structure of protein complexes; constructing contact maps (or RINs) from the distance matrices; dynamic network analysis, including vertex (residues, including ligands) degrees, edge (i.e., interactions) weights (or persistence time during MD), network clustering. The existing code package iGraph (in both Python and R) will be used by the intern. AFRL aims to generate an automated code package that can be adjusted for different protein and protein-complex systems. When completed, the final software package will be tested for multiple projects that are of DoD interest: REE-LanM binding affinity simulation, the ice-AFP interaction simulation, interactions between PFAS molecules and human serum albumin (HSA).

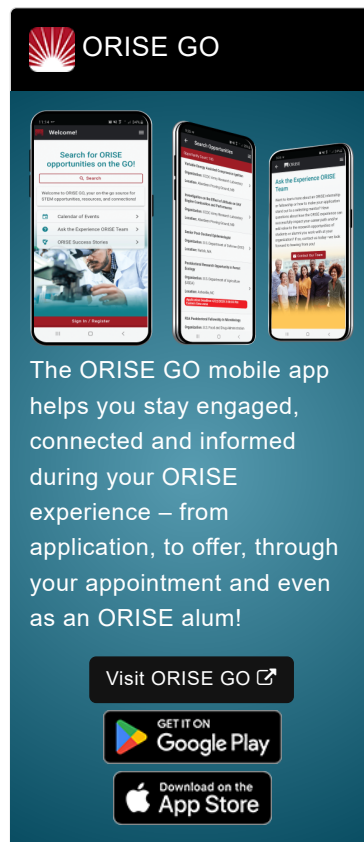
You will attend weekly workshops provided by AFRL/AFIT and surrounding institutions, such as resume and publication writing workshops, and will be encouraged to develop presentation skills via poster or oral presentations. You will participate in local meetings, presenting findings at computational group meetings, research team meetings, and branch-wide research meetings. Also, AFRL/RX holds a student poster session at the end of the summer. You will have an opportunity to attend technical talks at AFRL including weekly introductory technical talks in which research team leaders discuss ongoing projects in AFRL/RX, weekly in-house research updates, and visiting scientist lectures.

#### Why should I apply?

This fellowship provides the opportunity to independently utilize your skills and engage with experts in innovative ideas to move the proposed research forward.

**Where will I be located?** Wright-Patterson AFB, Ohio

**What is the anticipated start date?** June 2023

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

**What is the appointment length?**

This appointment is a summer research appointment. Appointments may be extended depending on funding availability, project assignment, program rules, and availability of the participant.

**What are the benefits?**

You will receive a stipend to be determined by the sponsor. Stipends are typically based on a participant's academic standing, discipline, experience, and research facility location. Other benefits may include the following:

- Health Insurance Supplement (*Participants are eligible to purchase health insurance through ORISE*)
- Relocation Allowance
- Training and Travel Allowance

**About ORISE**

This program, administered by Oak Ridge Associated Universities (ORAU) through its contract with the U.S. Department of Energy (DOE) to manage the Oak Ridge Institute for Science and Education (ORISE), was established through an interagency agreement between DOE and DoD. Participants do not enter into an employee/employer relationship with ORISE, ORAU, DoD or any other office or agency. Instead, you will be affiliated with ORISE for the administration of the appointment through the ORISE appointment letter and Terms of Appointment. Proof of health insurance is required for participation in this program. Health insurance can be obtained through ORISE. For more information, visit the [ORISE Research Participation Program at the U.S. Department of Defense](#).

**Qualifications** You should be a bachelor, master's, or doctoral student in a science or engineering field and is familiar with Python or R computer language and coding.

**Security Investigation:** Applicants should be able to pass a National Agency Check and Inquiries (NACI) security investigation should they be selected and accept the internship offer.

**Application Requirements**

A complete application consists of:

- Zintellect Profile
- Educational and Employment History
- Essay Questions (goals, experiences, and skills relevant to the opportunity)
- Resume (PDF)
- Transcripts/Academic Records - For this opportunity, an official transcript or copy of the student academic records printed by the applicant or by academic advisors from internal institution systems may be submitted. [Click here for detailed information about acceptable transcripts](#).
- One recommendation. Your application will be considered incomplete and will not be reviewed until one recommendation is submitted. We encourage you to contact your recommender(s) as soon as you start your application to ensure they are able to complete the recommendation form and to let them know to expect a message from Zintellect. Recommenders will be asked to rate your scientific capabilities, personal characteristics, and describe how they know you.

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You can always log back in to your Zintellect account and check the status of your application.

If you have questions, send an email to [USACE@orise.orau.gov](mailto:USACE@orise.orau.gov). Please list the reference code of this opportunity in the subject line of the email. Please understand that ORISE does not review applications or select applicants; selections are made by the sponsoring agency identified on this opportunity. All application materials should be submitted via the "Apply" button at the bottom of this opportunity listing. Please do not send application materials to the email address above.

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- Eligibility Requirements**
- **Citizenship:** U.S. Citizen Only
  - **Degree:** Bachelor's Degree, Master's Degree, or Doctoral Degree received within the last 60 months or currently pursuing.
  - **Overall GPA:** 3.00
  - **Discipline(s):**
    - **Chemistry and Materials Sciences** ([12](#))
    - **Computer, Information, and Data Sciences** ([17](#))
    - **Earth and Geosciences** ([21](#))
    - **Engineering** ([27](#))
    - **Life Health and Medical Sciences** ([48](#))
    - **Mathematics and Statistics** ([11](#))
    - **Physics** ([16](#))
    - **Science & Engineering-related** ([1](#))
  - **Age:** Must be 18 years of age
  - **Veteran Status:** Veterans Preference, degree received within the last 120 month(s).