Opportunity Title: 2025 HPCMP Summer Internship Program - Faculty: Graph-Grammar Based Machine Learning to Design Polymers for Applications
Opportunity Reference Code: HPCMP-FIX-010-F

Organization	U.S. Department of Defense (DOD)
Reference Code	HPCMP-FIX-010-F
How to Apply	Click on *Apply* at the bottom of the opportunity to start your application.
Application Deadline	6/13/2025 3:00:00 PM Eastern Time Zone
Description	

OAK RIDGE INSTITUTE FOR SCIENCE AND EDUCATION

About High Performance Computing Modernization Program (HPCMP)

The Department of Defense's (DoD) High Performance Computing Modernization Program (HPCMP) sponsors two summer research opportunities: the High-Performance Computing Internship Program (HIP) and the Faculty Immersion Experience (FIX). These 10-week experiences are offered in collaboration with more than a dozen DoD hosting organizations nationwide. Both programs seek to strengthen DoD and academic collaboration, enhance research capabilities, and encourage broader university-level participation in high-end computing.

About AFRL: Air Force Research Laboratory (AFRL) is a scientific research organization operated by the United States Air Force Materiel Command. AFRL is dedicated to leading the discovery, development, and integration of aerospace warfighting technologies, planning and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces.

Project: This project addresses the Air Force's critical need for materials that can withstand the extreme conditions of Arctic and Space environments. AFRL proposes a data-efficient machine learning framework that leverages graph grammar to inverse-design polymers with tailored thermal and mechanical properties. By interpreting molecules as graph networks, they will train a neural network to extract grammar rules for constructing and modifying molecular graphs, enabling the design of novel polymers optimized for specific Arctic and Space applications. This project will lead to the discovery of innovative materials that enable reliable operation in extreme environments, ultimately bolstering the Air Force's strategic advantage. Data-efficient framework that uses graph grammar & machine learning for inverse-designing polymers with targeted thermo-mechanical properties by tuning the polymer chemistry & architecture, catering to Artic & Space applications. The framework interprets molecules as graph networks, with atoms & bonds as nodes & edges, respectively. By predicting a set of grammar rules for constructing & modifying molecular graphs in a bottom-up fashion, new polymers can be designed to meet specific requirements. Project will involve:

- Developing virtual specimens with different polymer chemistry & network architecture using molecular dynamics (MD) simulations

- Model thermal (T_g, CTE) & mechanical (modulus, strength) properties @ 10K-300K regime

- For grammar extraction, train a neural network (NN) that can receive molecular graph containing nodes & edges/hyperedges as input

- Further augment the NN to learn sub-graphs made of nodes & edges/hyperedges, & extract immediate connectivities to establish grammar rules

What will I be doing?

Under the guidance of a mentor:
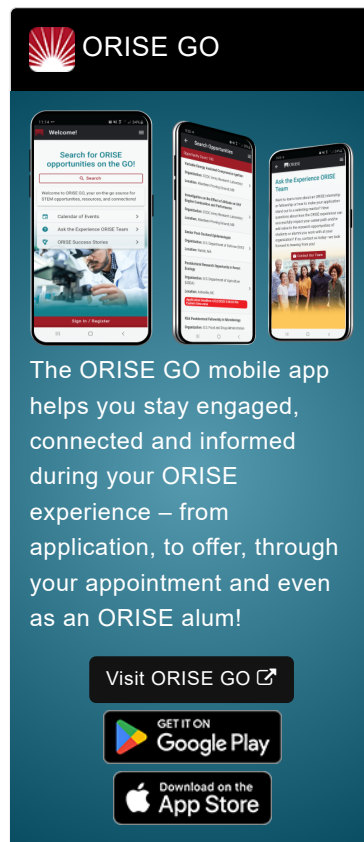
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- You will use molecular dynamics (MD) simulations to virtually fabricate a diverse array of polymeric systems, exploring the influence of chemical composition on properties like Tg & mechanical response. You will use DoD's HPC resources to accelerate these simulations & generate necessary data, to be utilized to construct a machine learning (ML) framework, guided by graph grammar, to predict & design polymers with tailored properties. Activities will further involve optimizing the accuracy & efficiency of the ML model and drafting a potential journal publication.

- You will engage in various professional development & networking opportunities, including AFRL's mission & research focus through RX101 seminars, tours of HPC facilities, weekly engagements in technical team meetings & collaboration with other AFRL researchers & visiting faculties.

-Given your knowledge in machine learning and atomistic simulations, it is expected that the technical aspects of the project will align well with your existing skill set. This project will present an exciting opportunity to deepen your knowledge of polymer science & expand your knowledge in applying computational methods to real-world materials challenges.

During this internship, you will:

- Learn from and collaborate with scientists and engineers at DoD facilities across the nation.
- Contribute to significant Research, Development, Test, Evaluation & Acquisitions Engineering activities.
- Develop critical skills and establish long-term connections.
- Receive financial support including a stipend and travel allowances.
- Gain a competitive advantage and improve long-term career opportunities.

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

What is the start date? June 2025

What is the appointment length? This appointment is a 10-week summer research appointment.

Provisions include:

- **Stipend:** Participants receive a monthly stipend to help defray living expenses during the appointment. Stipend rates are determined by HPCMP based on the participant's education level.
- **Dislocation Allowance:** A dislocation allowance may be provided for participants who relocate more than fifty miles, one-way, to the designated host site. This includes roundtrip domestic travel to/from the host location. Participant is responsible for and local transportation prior to arriving at the designated host site.
- **Professional Travel:** Participants may be eligible for reimbursement of pre-approved professional travel expenses related to the educational goals of the designated opportunity.
- **Health Insurance:** Participants may be eligible to enroll in ORISE health insurance to cover medical, dental and vision insurance.

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	Applicants must be full-time faculty from an accredited U.S. pre-college, college, or university in the science, technology, engineering or mathematics (STEM) field. Adjunct or visiting faculty are ineligible.

The faculty member should have a solid background in both the fundamental sciences and cutting-edge computational techniques. A Ph.D. in a relevant field such as Materials Science, Chemistry, or Physics and a strong foundation in computational materials science is necessary. This includes expertise in atomistic modeling techniques as well as proficiency in machine learning. Hands-on experience with molecular dynamics simulations, programming languages relevant to scientific computing, and familiarity with high-performance computing clusters are highly preferred. The faculty should thrive in collaborative research settings and be able to effectively communicate complex scientific concepts to a diverse audience.

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

A complete application consists of:

- Zintellect profile
- Educational and Employment History
- Curriculum Vitae (PDF)
- Salary Certification from your university

Submitted documents must have all social security numbers, student identification numbers, and/or dates of birth removed (blanked out, blackened out, made illegible, etc.) prior to uploading into the application system. All documents must be in English or include an official English translation. If you have questions, send an email to HPCMP@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.

Connect with ORISE...on the GO! Download the new ORISE GO mobile app in the Apple App Store or Google Play Store to help you stay engaged, connected, and informed during your ORISE experience and beyond!

Point of Contact	[Debbie](#)

Eligibility Requirements	- **Citizenship:** U.S. Citizen Only
	- **Degree:** Doctoral Degree.
	- **Discipline(s):**
	    ○ **Chemistry and Materials Sciences** (12 👁)
	    ○ **Computer, Information, and Data Sciences** (17 👁)
	    ○ **Earth and Geosciences** (21 👁)
	    ○ **Engineering** (27 👁)
	    ○ **Environmental and Marine Sciences** (14 👁)

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- **Mathematics and Statistics** (11 👁)
- **Physics** (16 👁)
- **Science & Engineering-related** (2 👁)
- **Age:** Must be 18 years of age
- **Veteran Status:** Veterans Preference, degree received within the last 120 month(s).