Opportunity Title: Computational Chemistry Research - Post-doctoral
Opportunity Reference Code: ERDC-EL-2025-0002

Organization U.S. Department of Defense (DOD)

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

Description The Environmental Laboratory (EL) is one of the seven laboratories of U.S. Army Engineer Research and Development Center (USACE-ERDC), which is the Army Corps of Engineers' integrated research and development (R&D) organization. EL provides solutions to environmental challenges for the U.S. Army, the Department of Defense and the Nation through environmental science and engineering research and development. Researchers in EL conduct research in ecosystem science and technology, environmental resiliency, environmental sensing, ecological modeling and forecasting, risk and decision science, environmentally sustainable material, systems biology, climate change, computational chemistry, environmental chemistry and environmental security.

What will I be doing?

Under the guidance of a mentor, you will gain knowledge by conducting research utilizing one or more computational chemistry approaches such as density functional theory, molecular dynamics simulations, and coarse-graining techniques. Knowledge of AI/ML in computational chemistry will be advantageous but not a necessary requirement. Research may cover one or more area relevant to fate and transport of different chemicals, structures and interactions of chemicals in the complex media, and development of multifunctional materials. Research may also focus on studying effects of hydration, adsorption, transport and diffusion of organic/inorganic species on some modeled surfaces at both the atomistic and coarse-graining level. You will engage in preparation of research results to be presented to the broader ERDC community, including, developing these results into publications to inform the broader scientific community through peer-reviewed journals and developing project ideas.

Where will I be located? Vicksburg, Mississippi

Why should I apply?

This internship provides the opportunity to independently utilize your skills and engage with experts in innovative ideas to move the proposed research forward. There are multiple opportunities available to engage in your applied research and evaluation interests.

What is the anticipated start date?

ERDC-EL is ready to make an appointment. Exact start date will be determined at the time of selection and in coordination with the selected candidates.

What is the length of the appointment?

This ORISE appointment is a full-time 12-month opportunity. Appointments may be extended depending on funding availability, project assignment, program rules, and availability of the participant.

What are the provisions?

You will receive a stipend to be determined by ERDC-EL. Stipends are typically based on the participant's academic standing, discipline, experience, and research facility location. Other

provisions 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 must have a PhD degree or graduating soon with knowledge in one or more of electronic structure methods, MD simulations, coarse-graining or computational rheology.

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

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 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.

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

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experience and beyond!

Point of Contact Debbie

Eligibility Requirements

- **Citizenship:** U.S. Citizen Only
- **Degree:** Doctoral Degree received within the last 60 months or currently pursuing.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12)
  - **Computer, Information, and Data Sciences** (16)
  - **Earth and Geosciences** (21)
  - **Engineering** (27)
  - **Environmental and Marine Sciences** (14)
  - **Life Health and Medical Sciences** (45)
  - **Mathematics and Statistics** (11)
  - **Physics** (16)
- **Age:** Must be 18 years of age