

Opportunity Title: Computer Science / Molecular Dynamics Modeling Summer

Internship

Opportunity Reference Code: ERDC-ITL-2023-0015

Organization U.S. Department of Defense (DOD)

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**How to Apply** Click on *Apply* at the bottom of the opportunity to start your application.

Description DEVCOM ARL, as an integral part of the Army Futures Command, is the Army's foundational research laboratory focused on operationalizing science to ensure overmatch in any future conflict. DEVCOM ARL shapes future concepts with scientific research and knowledge and delivers technology for modernization solutions to win in the future operating environment. (https://www.arl.army.mil/)

### What will I be doing?

Core-shell aluminum nanoparticles (nAI) are heavily studied via surface chemistry modification for high-energy fuel applications and are of great interest to the US Army. Experimental results have demonstrated that surface hydration plays a crucial role in nAl surface modification and subsequent nAl oxidation. As an Oak Ridge Institute for Science and Education (ORISE) participant, you will join a community of scientists and researchers in an effort to advance fundamental understanding of the interactions when amorphous and ?-phase alumina are exposed to water and how the resultant hydrolyzed alumina affects oxygen diffusion during different stages of nAl oxidation.

Under the guidance of a mentor, you will engage in a variety of research activities, including:

- · Developing practical supercomputing skills and gaining hands-on experiences through the use of supercomputers (ARL DSRC's Centennial and/or Scout)
- · Gaining profound knowledge, especially on novel energetics and applications of interest to the US Army and DOD
- · Opportunity to communicate with experimentalists who perform tasks that are immediately relevant to the summer project
- · Immediate feedback from researchers on the team and see how the modeling results fill the gap first-hand
- · interacting with many ARL researchers through seminars, Town Hall Meetings, and the corporate lab tours at ARL's APG and ALC sites for interns
- · Developing simulation models addressing challenging scientific questions that are difficult to answer via experimental approaches alone. At the end of the internship, the student will have multiple opportunities to present his/her work and will be trained to hone their scientific presentation skills
- · Presentation opportunities include the HIP Mini-session and oral or poster panels at the branch, division- and corporate-level as part of the 2023 ARL Summer Student Symposium

# 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.

## What is the anticipated start date? June 2023

Exact start date will be determined at the time of selection and in coordination with the selected candidate. Applications are reviewed on an ongoing basis and fellowships will be filled as qualified candidates are identified.



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## What is the appointment length?

This appointment is a ten-week research appointment, with the possibility to be renewed for additional research periods. 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 The qualified candidate will be a graduate student pursuing a Master's or Doctoral degree in Engineering, Computer Science, Mathematics or a related field.

> Highly competitive applicants will have education and/or experience in one or more of the following:

- Hands-on experiences in running molecular dynamics models using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software with appropriate interatomic potentials (for example ReaxFF) with Linux operating computers
- Sufficient writing and presentation
- · Previous experiences with nanoparticle related modeling
- · Ability to participate on-site with the team during the entire internship period

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 Please upload a copy of a transcript for your current or most

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recent degree program that meets the disciplinary qualifications of the opportunity. <u>Click here</u> <u>for detailed information about acceptable transcripts</u>.

One Recommendation. Your application will be considered incomplete and will not be
reviewed until one recommendation(s) 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. 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. Please list the reference code of this opportunity [ERDC-ITL-2023-0015] 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!

# 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.●)
  - Engineering (27 ●)
  - Life Health and Medical Sciences (48 )
  - Mathematics and Statistics (11 )
  - Physics (<u>16</u> ●)
  - Science & Engineering-related (1\_♥)
- Age: Must be 18 years of age
- **Veteran Status:** Veterans Preference, degree received within the last 120 month(s).

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