Opportunity Title: Theoretical Modeling of Sensing Materials for Autonomous Lab Development
Opportunity Reference Code: NETL-Postdoc-2026-Duan-2

Organization National Energy Technology Laboratory (NETL)

Reference Code NETL-Postdoc-2026-Duan-2

How to Apply A complete application consists of:

- An application, including academic history, work history experiences, and honors/awards
- Description of your goals, related experience, and related skills – refer to NETL's Core Competencies and ongoing projects when applicable
- Transcripts – Click here for detailed information about acceptable transcripts
- A current resume/CV, including academic history, employment history, relevant experiences, and publication list
- Two educational or professional recommendations
  You must provide contact information for at least two recommenders in your application. The first two recommendations received will be attached to your application for review by NETL. You may click the "send" (paper airplane) button to send the recommendation request email immediately after entering their information prior to submitting your application; if not, a request will automatically be sent when you submit your application. Your recommenders will receive an email with a subject line of "[Your Name] - ORISE Recommendation Request - [your email]", from Zintellect@orau.org. This email will include information on the opportunity to which you have applied, as well as a secure link to submit a recommendation for you for this application. If you ask the same person to submit a recommendation for you for multiple applications in Zintellect, they must click the unique link in each email request, but will be given the opportunity to copy over what they had previously submitted.

All documents must be in English or include an official English translation.

If you have questions before, during, or after you submit an application, you may reach out to NETLinfo@orau.org.

Application Tips

NETL values a combination of academic success, experience, and leadership potential as demonstrated in all aspects of your application. NETL's goal is to create, maintain, and support a diverse environment that encourages creative ideas and leadership. In the words of former Lab Director Brian Anderson, "our differences make us stronger and we're united in fostering inclusivity in all aspects of our research to drive innovation and deliver solutions for an environmentally sustainable and prosperous energy future." In your application, show us who you are!

To increase your chances of being selected for an appointment, we recommend:

1. Tailoring your responses to align with the project. What parts of the

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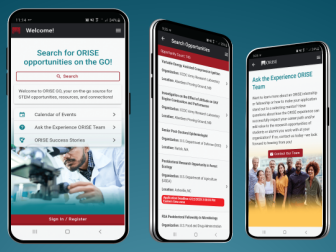

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project are most interesting to you?
2. Spending sufficient time on your essay responses and your resume. Give yourself time to review your writing!
3. Ensuring that everything you submit is grammatically correct and clearly expressed.

Application Deadline 12/31/2026 11:59:59 PM Eastern Time Zone

Description The National Energy Technology Laboratory's (NETL's) record of success has been built on understanding the future of energy and the technologies required to make that future possible. We've long touted our success in developing the technologies that took on acid rain in the 1970s and mercury in the early 2000s.

Program Goals

The NETL Postdoctoral Research Fellowship Program (Postdoc) is a high-intensity program designed to identify recent Doctoral graduates of high promise and to foster advanced skill development. It allows the postdoc to systematically outline career goals and helps provide the means of achieving these goals. NETL principal investigators and leads serve as mentors to postdoctoral participants during the program. This interaction affords the postdoc a unique opportunity to develop critical skills needed to become an independent professional.

The program goals include providing the opportunity to participants to:

- Develop skills and knowledge in their field of study
- Engage with new areas of basic and applied research
- Network with world-class scientists
- Exchange ideas and skills with the Laboratory community
- Use state-of-the-art equipment
- Contribute to answers for today's pressing scientific questions
- Collaborate with the broader scientific and technical communities

Project Details

Through the Oak Ridge Institute for Science and Education (ORISE), this posting seeks a post-Doctoral researcher to engage in projects with the Research Innovation Center (RIC) at the National Energy Technology Laboratory (NETL) in the area of Autonomous Lab for Sensing Materials Development under the mentorship of Yuhua Duan. This project will be hosted at the NETL Pittsburgh, PA campus.

Although material modeling with artificial Intelligence/machine learning (AI/ML) applications and experimental instrumental measurements have been advanced significantly in sensing technology development, the synthesis, testing and characterization in current research labs still require human operation and take a long time for relatively repetitive steps to validate findings from theoretical calculations. Autonomous labs or self-driving laboratories can combine AI and automatic robotic operation to intelligently conduct experiments and accelerate sensing materials discovery and development. By leveraging NETL existing and strong competencies, the objective of the overarching project is to develop an Autonomous Lab for Sensing Materials.

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The learning objectives for this project are: (1) use atomistic simulation software and AI/ML techniques on sensing materials database development, (2) analyze the modeling results, and (3) learn oral and writing skills for preparing technical reports and giving scientific presentations.

Stipend: The selected participant will receive a monthly stipend commensurate with educational level and experience.

- Post-Doctoral stipend is $8126 per month.

Program Requirements: To document the effectiveness of the program, participants are required to submit a pre-appointment and post-appointment survey, as well as a reflection on their appointment experience when they renew or end their appointment. The reflection should summarize their project(s), additional activities, and overall experience. Details are provided as the appointment end date approaches.
Participants may also have the opportunity to contribute to manuscripts, journal articles, book chapters, conference presentations, posters, patents, and other publications as a part of their appointment. Such achievements should also be reported to ORISE; additional details are provided after an offer has been accepted.

The National Energy Technology Laboratory (NETL), part of the U.S. Department of Energy (DOE) national laboratory system, is owned and operated by the DOE. NETL supports the DOE mission to advance the energy security of the United States. This is an educational opportunity offered by NETL and administered by the Oak Ridge Institute for Science and Education. Participants in the program are not considered employees of NETL, DOE, the program administrator, or any other office or agency.

Qualifications The ideal candidate would have some, but not necessarily all, knowledge of and skills in:

- PhD in Physics or Chemistry
- Experience with computational physics, chemistry, and materials science.
- Research experience involving density functional theory and ML simulations
- Familiarity with software packages such VASP, CP2K, Gaussian, Scikit-learn, TensorFlow, SciML, etc., as well as database development.

It is recognized that not all applicants will have knowledge and experience in all of these areas. This opportunity will provide exposure to/interaction with technical experts in several of these areas.

To be eligible, you must either:

- have received a Doctoral degree within the last five years *or* be currently enrolled in a Doctoral degree program and complete the degree prior to the appointment start date.

Point of Contact Jordan

Eligibility

- **Degree:** Doctoral Degree received within the last 60 months or currently

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Requirements

pursuing.

- **Discipline(s):**
  - **Business** (11 👁)
  - **Chemistry and Materials Sciences** (12 👁)
  - **Communications and Graphics Design** (6 👁)
  - **Computer, Information, and Data Sciences** (17 👁)
  - **Earth and Geosciences** (21 👁)
  - **Engineering** (29 👁)
  - **Environmental and Marine Sciences** (14 👁)
  - **Life Health and Medical Sciences** (51 👁)
  - **Mathematics and Statistics** (11 👁)
  - **Other Non-Science & Engineering** (13 👁)
  - **Physics** (16 👁)
  - **Science & Engineering-related** (2 👁)
  - **Social and Behavioral Sciences** (30 👁)
- **Age:** Must be 18 years of age

Affirmation

I certify that I attend or attended a regionally accredited college or university and:

- Have an earned a Doctoral degree no more than five years before the date of application.

  OR

- Will receive a Doctoral degree by the appointment start date