

**TITLE:** Post-Doctoral Researcher in High-Throughput Computational Screening of CO<sub>2</sub> Capture Materials

**DEPARTMENT:** U.S. Department of Energy

**AGENCY:** National Energy Technology Laboratory (NETL)

**LEVEL:** Post-doctoral

**POSITION INFORMATION:** Full-time, one year appointment, with opportunity for renewal.

**DUTY LOCATION:** Pittsburgh, Pennsylvania

**WHO MAY BE CONSIDERED:** United States Citizens, LPRs, & Foreign Nationals with appropriate authorization and approval.

**SUMMARY:**

A highly motivated post-doctoral associate is sought to participate in the development of a new, innovative high-throughput computational tool suite for the prediction of materials properties in carbon capture materials. Specifically, the goals of this project will be to simulate a large database of materials and their associated carbon-capture-relevant properties and coordinate with the toolset of the Carbon Capture Simulation Initiative (CCSI) in order to optimize on carbon capture material and process simultaneously.

Specifically the selected applicant will:

- Develop algorithms for the high-throughput simulation of the properties of materials
- Develop methods for data storage and the rapid analysis of large data sets
- Create standards for programming, maintain and administer a growing simulation code
- Collaborate within NETL as well as with University partners

To be successful in this position, you must have:

- A doctorate (or will shortly obtain one) in computer science, physics, chemistry, mathematics, engineering or a related discipline
- An outstanding level of motivation and self-sufficiency
- Demonstrated experience with scientific programming on a large scale
- Knowledge of and research experience with high-throughput computational methods, optimization, machine learning, or similar fields
- Experience with database design, maintenance, and analysis
- Excellent verbal and written English communication skills
- The ability to represent our research team effectively both internally and externally, including at conferences or other meetings

This work will be co-mentored by Dr. Jan Steckel (NETL) and Professor Chris Wilmer (University of Pittsburgh). NETL is part of the U. S. Department of Energy's national laboratory system, supports the DOE mission to advance the energy security of the United States, and is currently funding the development of advanced carbon dioxide (CO<sub>2</sub>) capture technologies that have the potential to provide capture with improved performance and reduced cost.

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry, and academic institutions that is developing, demonstrating and deploying state-of-the-art computational modeling and simulation tools to accelerate the development of carbon capture

technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants.

NETL's Oak Ridge Institute for Science and Education (ORISE) Program is administered by Oak Ridge Associated Universities and provides opportunities for undergraduate students, recent graduates, graduate students, postdoctoral researchers, and faculty researchers to perform energy-related research at NETL.

#### **HOW TO APPLY:**

Applicants should apply through the Oak Ridge Institute for Science and Education (ORISE) program. The ORISE Program provides opportunities for undergraduate students, recent graduates, graduate students, postdoctoral researchers, and faculty researchers. NETL utilizes the ORISE program to support research and work within NETL's Office of Research & Development.

- Interested applicants should complete the online application at <http://www.ornl.gov/netl/>
- In the online application **list Jan Steckel as your requested mentor.** This will associate your application with this job posting.
- If you have additional questions please contact Nancy Andres, [Nancy.Andres@NETL.DOE.GOV](mailto:Nancy.Andres@NETL.DOE.GOV), who is the NETL ORISE program contact.