

Opportunity Title: PostDoc Researcher in Code Devlpmt for High-Throughput

Comp Screening of CO2 Capture Mat'l's

Opportunity Reference Code: NETL-2015-09-4-Steckel

Organization National Energy Technology Laboratory (NETL)

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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, who is the NETL ORISE program contact.

Application Deadline 6/9/2016 12:00:00 AM Eastern Time Zone

Description 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, we seek a candidate with significant experience in software development, optimization of scientific programs, and experience with piping and other automation methods. 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:

- Analyze and optimize simulation code for performance
- Develop methods for the automation of simulations
- 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



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- 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 (CO₂) 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.

Qualifications • Applicants must be U.S. Citizens or approved Foreign Nationals

Eligibility • **Degree:** Doctoral Degree.

Requirements • **Discipline(s):**

- **Chemistry and Materials Sciences** ([12](#) )
- **Communications and Graphics Design** ([1](#) )
- **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** ([10](#) )
- **Other Non-Science & Engineering** ([13](#) )
- **Physics** ([16](#) )
- **Science & Engineering-related** ([1](#) )
- **Social and Behavioral Sciences** ([27](#) )