

TITLE: Post-Doctoral Researcher – Molecular Simulations - CO₂ 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 the possibility of extension.

DUTY LOCATION: Pittsburgh, Pennsylvania

WHO MAY BE CONSIDERED: United States Citizens, LPRs, & Foreign Nationals with qualifying documentation and approval.

SUMMARY:

A highly motivated post-doctoral associate is sought to participate in the development and expansion of an in-house molecular dynamics and Monte Carlo code, and the application of new methodologies for the prediction of the properties of novel CO₂ capture materials. Specifically, the goals of this project will be to:

- (1) Add new capabilities to the existing molecular dynamics and Monte Carlo codes, (for example, the implementation of non-equilibrium dynamics) and
- (2) Apply existing and new methodologies in molecular simulation to the calculation of properties of novel carbon capture materials.

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
- Research experience with molecular dynamics simulations and/or Monte Carlo methods as applied to atomistic modeling
- Fluency and demonstrated experience coding in FORTRAN or a similar language
- Experience with parallel code development and script languages
- Experience developing advanced molecular simulation methodologies
- Demonstrated experience with force field development
- Excellent verbal and written English communication skills
- The skills necessary 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 Dr. Wei Shi (NETL/AECOM). NETL is part of the U.S. Department of Energy's national laboratory system, supporting the DOE mission to advance the energy security of the United States. NETL 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.

NETL's Oak Ridge Institute for Science and Education (ORISE) Program is administered by ORAU 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, who is the NETL ORISE program contact.