



NREL's Mission

NREL develops renewable energy and energy efficiency technologies and practices, advances related science and engineering, and transfers knowledge and innovations to address the nation's energy and environmental goals.

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Equal Opportunity

NREL is an equal opportunity employer committed to diversity and a drug-free workplace.

National Renewable Energy Laboratory 15013 Denver West Parkway, Golden, CO, 80401

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

The National Renewable Energy Laboratory (NREL), located in beautiful Golden, Colorado, is a leader in the U.S. Department of Energy's effort to secure an energy future for the nation that is environmentally and economically sustainable.

Postdoctoral Researcher - Computational Modeling of Combustion R1382

Job Summary:

The National Renewable Energy Laboratory has an opening for a postdoctoral researcher in the National Bioenergy Center. Recent PhD graduates are invited to apply to this postdoctoral position to aid with the development of predictive computational models for combustion research, which will focus on identifying bio-derived fuel candidates for next generation engines.

Primary Duties Include:

- Ability to perform ab initio calculations using standard software packages (e.g. Gaussian) with little to no oversight and interact with modeling and experimental collaborators at NREL and other institutions.
- Incorporate machine learning methodologies toward the development of rapid predictive and screening tools.
- Perform kinetic modeling of combustion reactions using RRKM and/or ChemKin.
- Effectively communicate and interact with scientists and engineers to define the requirements of the simulations/models. Obtain necessary input data for simulations, and provide meaningful interpretation of modeling results to guide experiments, operations, and engineering designs.
- Disseminate knowledge through publications in technical journals and presentations at conferences, symposia, and review meetings.
 Provide reports on technical work and input to technical publications and presentations.
- Work with management and senior staff to plan and design projects, determine technical objectives, and interact with and provide regular project reports to government and/or industrial clients.

The successful candidates will have the following skills and experience:

- Well-versed in quantum chemistry and related softwares (e.g. Gaussian).
- Strong background in combustion chemistry/physics, modeling and kinetics (preferably with an emphasis on bio-fuels applications)
- Demonstrated experience in performing simulations studies that inform and collaborate with experimental projects.
- Experience in software development and coding.

- Ability to work independently or in teams and to deliver high-quality results within aggressive timelines.
- Excellent technical writing, interpersonal, and communication skills.
- Troubleshooting and problem-solving skills.
- Recent (within past three years) PhD in Chemistry, Chemical Engineering or related field with a focus on computational modeling.
- Dedication to a safe and clean work environment

Preferred Qualifications:

 Strong publication record. Applicants should be fluent in at least one scientific programming environment (Python, R, Matlab, Fortran, C, etc.). A strong background in mathematics and computational statistics, DFT calculations, and chemical kinetics are essential. Experience with machine

learning training/validation/testing paradigm is highly preferred. In-depth knowledge of combustion chemistry/physics is critical.

Required Education, Experience, and Skills:

Must be a recent PhD graduate within the last three years.

Submission Guidelines:

Please note that in order to be considered an applicant for any position at NREL you must submit an application form for each position for which you believe you are qualified. Applications are not kept on file for future positions. Please include a cover letter and resume with each position application.

EEO Policy:

NREL is dedicated to the principles of equal employment opportunity. NREL promotes a work environment that does not discriminate against workers or job applicants and prohibits unlawful discrimination on the basis of race, color, religion, sex, national origin, disability, age, marital status, ancestry, actual or perceived sexual orientation, or veteran status, including special disabled veterans.

NREL validates right to work using E-Verify. NREL will provide the Social Security Administration (SSA) and, if necessary, the Department of Homeland Security (DHS), with information from each new employee's Form I-9 to confirm work authorization.

To Apply: www.nrel.gov/careers R1382

For questions: Marlo Hughen, Sr. Recruiter: Marlo.Hughen@NREL.gov