

Research Associate Chemical Science and Machine Learning

Job ID 2411 Date posted 12/03/2020

Brookhaven National Laboratory is a multipurpose research institution funded primarily by the U.S. Department of Energy's Office of Science. Located on the center of Long Island, New York, Brookhaven Lab brings premier facilities and expertise to the most exciting and meaningful questions in basic and applied science—from the birth of our universe to the sustainable energy technology of tomorrow. We operate state-of-the-art large-scale facilities for studies in physics, chemistry, biology, medicine, applied science, and a wide range of advanced technologies. Brookhaven Lab employs nearly 3,000 scientists, engineers, and support staff, and engages more than 4,000 visiting researchers from around the world each year. Our award-winning history, including seven Nobel Prizes, stretches back to 1947, and we continue to unravel mysteries from the nanoscale to the cosmic scale. Brookhaven Science Associates, a nonprofit applied science and technology organization, operates Brookhaven Lab for the U.S Department of Energy.

Organizational Overview

The CFN is a DOE-funded national scientific user facility, offering users a supported research experience with top-caliber scientists and access to state-of-the-art instrumentation. The CFN mission is advancing nanoscience through frontier fundamental research and technique development, and is the nexus of a broad collaboration network. Each year, CFN staff members support the research of nearly 600 external facility users.

Three strategic nanoscience themes underlie the CFN scientific facilities: The CFN fosters research on complex self-assembly processes, for building new ways of constructing **Self-Assembled Nanomaterials by Design**. The CFN supports state-of-the-art techniques for designing **Nano-Architectures** to improve the performance of materials. The CFN develops and provides advanced capabilities for studies of **Nanomaterials in Operando Conditions**, for characterizing materials and reactions at the atomic scale in real-world environments.

Position Description

The CFN is seeking an exceptional Postdoctoral Research Associate to lead research on a new project focused on building an interpretable machine learning framework coupled with transient kinetics spectroscopy to transform the way surface reaction mechanisms are derived. You will develop new data analytics tools with the latest neural network models and apply them to the rich data generated from emerging transient kinetics experiments at CFN and the Chemistry Department. You will use this cutting-edge digital apparatus to study hydrogenation reactions on metal surfaces and explore dynamic heterogeneous catalysis to dramatically increase reactivity. You will be under the supervision of CFN scientist Qin Wu, and work closely with CFN scientists Xiaohui Qu and Anibal Boscoboinik.

Position Requirements

Required Knowledge, Skills, and Abilities:

You are qualified for this Research Associate position if:

- You earned a Ph.D. in an appropriate discipline (Chemistry, Chemical Engineering, Physics, or Materials Science) within the past five years;
- You are familiar with microkinetic modeling of heterogeneous catalysis;
- You have computer coding experience in Python or other programming languages;
- You have demonstrated an ability to communicate effectively by writing scientific papers and giving technical presentations;
- You are committed to fostering an environment of safe scientific work practices.

Preferred background and experience:

You are well-matched to this position if:

- You have knowledge of numerical methods for differential equations;
- You have experience using deep neural networks for scientific investigations;
- You have studied mechanisms of chemical reactions on surfaces;
- You have basic knowledge of surface science experiments;
- You work effectively in a collaborative team to tackle challenging scientific problems.

BNL policy requires that research associate appointments be made to individuals who have received their doctorate within the past five years.

At Brookhaven National Laboratory we believe that a comprehensive employee benefits program is an important and meaningful part of the compensation employees receive. Our benefits program includes, but is not limited to:

- Medical, Dental, and Vision Care Plans
- Flexible Spending Accounts
- Paid Time-off and Leave Programs (vacation, holidays, sick leave, paid parental leave)
- 401(k) Plan
- Flexible Work Arrangements
- Tuition Assistance, Training and Professional Development Programs
- Employee Fitness/Wellness & Recreation: Gym/Basketball Courts, Weight Room, Fitness Classes, Indoor Pool, Tennis Courts, Sports Clubs/Activities (Basketball, Ping Pong, Softball, Tennis)

We invite you to consider working at Brookhaven Lab. To be considered for this position, apply online at www.bnl.gov and click Jobs, then sort by jobID and apply to job#.

Brookhaven National Laboratory is an equal opportunity employer committed to ensuring that you receive full consideration for employment. No one will be discriminated against on the basis of race, color, religion, sex, sexual orientation, national origin, age, disability, or protected veteran status.

BNL takes affirmative action in support of its policy and to advance in employment individuals who are minorities, women, protected veterans, and individuals with disabilities.

Brookhaven National Laboratory (BNL) is an equal opportunity employer that values inclusion and diversity at our Lab. We are committed to ensuring that all qualified applicants receive consideration for employment and will not be discriminated against on the basis of race, color, religion, sex, sexual orientation, gender identity, national origin, age, status as a veteran, disability or any other federal, state or local protected class.

BNL takes affirmative action in support of its policy and to advance in employment individuals who are minorities, women, protected veterans, and individuals with disabilities. We ensure that individuals with disabilities are provided reasonable accommodation to participate in the job application or interview process, to perform essential job functions, and to receive other benefits and privileges of employment. Please contact us to request accommodation.

*VEVRAA Federal Contractor

Brookhaven employees are subject to restrictions related to participation in Foreign Government Talent Recruitment Programs, as defined and detailed in United States Department of Energy Order 486.1A. You will be asked to disclose any such participation at the time of hire for review by Brookhaven. The full text of the Order may be found at: https://www.directives.doe.gov/directives-documents/400-series/0486.1-BOrder-a/@_@images/file