

Postdoctoral Research Associate Materials Science

Theory & Computation Group
Center for Functional Nanomaterials
Brookhaven National Lab
Group Leader: Mark S Hybertsen
Application through the job portal on-line at www.bnl.gov

Job ID 1667

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 world-class facilities and expertise to the most exciting and important questions in basic and applied science—from the birth of our universe to the sustainable energy technology of tomorrow. We operate cutting-edge large-scale facilities for studies in physics, chemistry, biology, medicine, applied science, and a wide range of advanced technologies. The Laboratory's almost 3,000 scientists, engineers, and support staff are joined each year by more than 4,000 visiting researchers from around the world. 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, and everything in between. Brookhaven is operated and managed by Brookhaven Science Associates, which was founded by the Research Foundation for the State University of New York on behalf of Stony Brook University, and Battelle, a nonprofit applied science and technology organization.

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 Synthesis by Nanomaterial Assembly. The CFN researches and applies platforms for state-of-the-art techniques for Accelerated Nanomaterial Discovery for target structure and functionality. The CFN develops and utilizes 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 using theory, computation and deep data analysis methods to unravel key structure motifs in nanostructured materials and the chemical reactions catalyzed by those materials. CFN researchers are actively pursuing projects directed to several examples of catalytic materials with a focus on control of reaction sites at the atomic scale. In this research, you will work on theory or data analytics driven projects and on questions directly tied to experimental data under the supervision of Mark Hybertsen and jointly with other members of the Theory and Computation Group depending on specific project goals. You will also have the opportunity to work closely with CFN staff scientists performing

experiments with state-of-the-art *in situ* and *operando* facilities based on X-ray absorption, photoemission, transmission electron microscopy, and/or infrared spectroscopy.

Position Requirements

Required Knowledge, Skills, and Abilities:

You are qualified for this Research Associate position if:

- You have earned a Ph.D. in an appropriate discipline (Physics, Chemistry, Materials Science, or a related engineering discipline) within the past five years or will complete your degree prior to starting;
- You have used Density Functional Theory based computational tools, widely applied in the study of materials and molecules, as a primary tool in your research projects;
- You have working experience with programming, script development, and/or tools for automating computational work;
- You work effectively in a collaborative team to tackle challenging scientific problems, particularly the application of theory and simulation to understand experimental results;
- 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 working knowledge of chemical reaction mechanisms;
- You have knowledge of deep learning methods;
- You are interested in learning how to use physical theory and computation together with deep learning methods;
- You can work independently within the team;
- You communicate effectively, both verbally and also through writing;

Employment benefits

At Brookhaven Lab, we believe comprehensive employee benefits are a meaningful part of employee compensation. Our benefits program includes:

- Medical Plans
- Vacations
- Holidays
- Dental Plans
- Life Insurance
- 401(k) Plan
- On site swimming pool, weight room tennis courts, and other employee benefits

Application

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 job ID and apply.

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.

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