SLAC NATIONAL ACCELERATOR LABORATORY
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Operated by Stanford University for the U.S. Department of Energy

Postdoctoral Scholar in Computational X-ray Spectroscopy for Electrocatalysis

The **Stanford Synchrotron Radiation Lightsource (SSRL)** at **SLAC National Accelerator Laboratory** invites applications for a **Postdoctoral Scholar** position focusing on **computational X-ray spectroscopy and electrocatalysis modeling**. This role combines advanced simulation techniques and computational chemistry to interpret X-ray absorption spectra and model catalytic systems, contributing to forefront electrocatalysis research at the intersection of theory and experiment.

The successful candidate will use **OCEAN**, **ORCA**, and **first-principles DFT methods** to simulate and interpret X-ray spectra, directly supporting the understanding of catalytic processes under operando conditions. Additionally, the candidate will optimize **geometry structures for extended systems and surfaces**, model **adsorption processes**, and calculate **Pourbaix diagrams** to evaluate the stability of candidate structures under electrochemical conditions. A strong focus will also be placed on streamlining computational workflows for **high-performance computing (HPC) facilities**, such as **NERSC**, **S3DF**, and **Sherlock**, enabling high-throughput simulations to match the scale and complexity of modern experimental data.

This position plays a critical role in furthering **SSRL's experimental advances**, enabling the interpretation of **high-throughput operando data**, and contributing to the effort to develop transformative catalytic and energy conversion technologies.

Position Overview

The successful candidate will:

- Perform **first-principles simulations** of X-ray absorption, emission, and inelastic scattering spectra using **OCEAN** (and/or **ORCA)**, with a focus on catalysis-relevant materials.
- Optimize **extended system geometries**, including surfaces with adsorbates, using **density functional theory (DFT)**.
- Model catalytic surfaces and identify stable structures for electrocatalytic reactions under realistic conditions.
- Calculate **Pourbaix diagrams** to predict the stability of materials and reaction intermediates under varying electrochemical potentials and pH.
- Develop, optimize, and automate computational workflows on supercomputing facilities (**NERSC**, **S3DF**, **Sherlock**, etc.) to enable high-throughput simulations of complex systems.
- Collaborate closely with experimentalists to interpret high-throughput operando data and guide experimental designs.
- Contribute to the understanding of **CO_2 reduction pathways**, **HER**, and **OER mechanisms** by modeling reaction intermediates, transition states, and catalytic dynamics.

Key Attributes

We are seeking candidates who:

- Have a deep understanding of **electronic structure theory** and extensive experience in computational modeling of materials.
- Thrive in **data-driven and multidisciplinary research environments**, bridging theoretical simulations and experimental findings.
- Are motivated to address fundamental challenges in catalysis and spectroscopy by developing scalable, innovative approaches to modeling complex systems.
- Are enthusiastic about streamlining computational workflows for efficient use of high-performance computing resources.

Qualifications

- **Required**:
  - Ph.D. in **Physics, Chemistry, Materials Science**, **Engineering**, or a related field.
  - Expertise in **first-principles calculations** (e.g., DFT, TDDFT) and electronic structure theory.
  - Experience with X-ray spectroscopy simulation codes such as **OCEAN**, **ORCA**, or similar tools.
  - Demonstrated ability to perform **geometry optimizations** for extended systems and surfaces, including adsorbate modeling.
  - Proven track record in calculating and interpreting **Pourbaix diagrams** for electrocatalytic materials.
  - Programming skills in **Python, C++**, **or Matlab** with experience in developing computational workflows.
  - Experience with high-performance computing (HPC) environments for large-scale simulations.
  - Strong publication record in computational spectroscopy or materials modeling.
- **Preferred**:
  - Familiarity with **CO_2 reduction**, **HER**, and **OER** reaction mechanisms.
  - Knowledge of advanced workflow optimization for HPC facilities, including NERSC and other supercomputing platforms.
  - Experience collaborating with experimental scientists in multidisciplinary teams.

Why Join Us?

This role offers:

- An opportunity to lead the development of computational techniques that bridge theory and experiment, enabling transformative insights into catalysis and energy conversion processes.

- Access to **world-class computational and experimental facilities** at SLAC National Accelerator Laboratory, including cutting-edge supercomputing resources.
- A collaborative, high-performance research environment where you can contribute to groundbreaking advances in spectroscopy and materials science.
- The chance to work on **well-funded collaborative efforts**, focusing on impactful energy conversion and storage technologies.

Appointment Terms

- This is a 1+1-year position, with the possibility of renewal based on performance and funding availability.
- The position is based at SLAC National Accelerator Laboratory, Menlo Park, CA.

How to Apply
Please submit:

1. A cover letter detailing your research experience and suitability for this role.
2. A curriculum vitae, including a list of publications.
3. Contact information for three professional references.

Applications will be reviewed on a rolling basis until the position is filled. For inquiries, contact **Dr. Dimosthenis Sokaras** at **dsokaras@slac.stanford.edu**

About SLAC
At SLAC National Accelerator Laboratory, our mission is guided by five core values:

- **Excellence**: Committing to the highest standards in safety, science, and operations.
- **Integrity**: Acting with honesty, accountability, and transparency.
- **Collaboration**: Fostering teamwork to achieve shared goals and maximize impact.
- **Respect**: Valuing the contributions of every individual and maintaining a welcoming culture.
- **Creativity**: Embracing new ideas and innovation with optimism and determination.

These values define who we are and drive our success in advancing scientific discovery and technological innovation.