



Postdoctoral Research Associate Position in Computational Crystallography

The SSRL (Stanford Synchrotron Radiation Lightsource) Directorate at SLAC National Accelerator Laboratory invites applications for a Postdoctoral Research Associate to join a DOE-funded project titled PECS: Protein Ensemble Compound Screening for Biothreat Response and Drug Discovery.

This project seeks to expand the capabilities of the **Macromolecular Crystallography Group** at SSRL, enabling users to routinely capture, extract, and apply protein ensemble information from X-ray diffraction data using novel machine learning (ML), advanced simulation, and high-performance computing (HPC) techniques.

The successful candidate will specifically lead the **Dynamics Optimized High Throughput Workflows** component of the PECS project. This involves developing automated, real-time pipelines and advanced algorithms to autonomously steer and optimize time-resolved, compound screening, and/or other high throughput crystallography experiments.

This role offers a unique opportunity to gain expertise in the intersecting disciplines of structural biology, macromolecular crystallography, data science and high-performance computing at a DOE light source user facility.

Key responsibilities of this role are focused on software architecture, algorithm development, and data analysis:

- **Algorithmic Steering:** Develop and benchmark advanced algorithms for automatic experiment steering, using real-time feedback from supervised ML models to optimize beamtime and maximize the targeted detection of structural intermediates.
- **Forward Simulations:** Adapt existing forward diffraction simulation pipelines to produce model training data for various experimental scenarios.
- **HPC Implementation:** Implement and optimize GPU-accelerated diffraction data reduction and analysis algorithms to achieve ultra-fast processing times, further enabling real-time decision-making during experiments.
- **Software Integration:** Design and implement the software architecture required to integrate laboratory automation systems and beamline control with the real-time data analysis and experiment steering routines.
- **Scientific Validation & Collaboration:** Collect, analyze, and publish time-resolved compound screening data in collaboration with beamline staff and key beamline users.
- **Dissemination:** Write a high-impact paper promoting the new SSRL resource, publish key results, and present research at a common crystallography conference.

Required qualifications

- Ph.D. in a relevant computational or experimental field (e.g., Physics, Computational Chemistry, Computer Science, Bioinformatics, Structural Biology, or a related discipline)

completed within the last three years, or confirmation of Ph.D. requirements completion prior to the start date.

- Strong foundation in structural biology, macromolecular crystallography, or a related discipline, as demonstrated through publication history.
- Extensive experience with Python and professional software development practices (including test-driven code development and version control).
- Familiarity with computational methods and concepts in optimization and machine learning.
- Excellent data processing, analysis, organization, and interpersonal skills, with the ability to work effectively in a large, multi-disciplinary team.
- Proficiency working in a Unix shell environment

Preferred qualifications

- Familiarity with AI/ML frameworks such as PyTorch, TensorFlow, or JAX.
- Demonstrated experience/interest with GPU programming (e.g., CUDA, OpenCL).
- Prior experience with diffraction data analysis software (e.g., DIALS, XDS, Phenix).
- Knowledge of SLURM or similar for job management in a compute cluster environment.
- Experience or strong interest in beamline operations or scientific user facilities.

This is a **fixed-term staff position**, expected to be a **2-year appointment** with the possibility of extension up to a full 32 months, contingent upon project needs and funding.

Application materials should include a **cover letter**, a **statement of research area** including a summary of accomplishments, a **curriculum vitae (CV)**, a **list of publications**, and names of **three references for future letters of recommendation**.

Please email all application materials to Dr. Derek Mendez; dermen@slac.stanford.edu

SLAC is a U.S. Department of Energy (DOE) laboratory operated by Stanford University and based in Menlo Park, CA. The **Macromolecular Crystallography Group** is part of the Structural and Molecular Biology division of the SSRL directorate.