



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.