

XFEL Crystallography Specialist - 96195
Division: MB-Molecular Biophys & Integ Bio

Berkeley Lab's Molecular Biophysics & Integrated Bioimaging (MBIB) Division is looking for a XFEL Crystallography Specialist as part of a group focusing on scientific software for X-ray crystallography.

The next decade of structural biology at X-ray free-electron lasers (XFELs) will include groundbreaking advances in time-domain crystallography, performed at room temperature to preserve biologically relevant dynamic mechanisms. Considering the anticipated scale of these data, we have ambitious collaborations with experimental groups targeting structural biology, light source science groups at facilities such as the Linac Coherent Light Source (LCLS), and high-performance computing groups at national supercomputing facilities such as the National Energy Research Scientific Computing Center (NERSC), also located in Berkeley.

The group's projects will include 1) Photosystem II, discovering the sequence of redox events leading to the release of molecular oxygen, using a combination of time-resolved crystallography and X-ray emission spectroscopy, and 2) Examining the electronic environment of metalloenzyme catalytic metals, with detection based on anomalous scattering; 3) outreach and training of XFEL scientists.

In this exciting role, you will be positioned to launch into High Performance Computing (HPC) careers at light source or other experimental facilities.

What You Will Do:

- Participate as the Crystallography Specialist on multidisciplinary teams performing XFEL experiments.
- Take the lead on developing and testing software for X-ray free-electron laser (XFEL) crystallography, using our previously developed packages (cctbx.xfel and dials) as a starting point.
- Develop a deep understanding of the hardware available for Exascale computing (including Perlmutter, Aurora and Frontier), along with GPU accelerators.
- Work at the interface between supercomputer design teams, computer science groups, LCLS beamline scientists, and X-ray crystallography user groups.
- Derive new algorithms to adapt to heterogeneous experimental designs.
- Deliver new features on time and in support of structural biology.
- Deliver U.S. Department of Energy (DOE)-mandated software development milestones on time, including tested code checked in to repositories, accompanied by written reports.
- Write one first-author paper per year in scientific publications.
- Present work at conferences, and continuously communicate results to several collaborating groups.

What s Required:

- A minimum of 3 year of relevant experience beyond the highest customary degree in Biophysics, Bioinformatics, Mathematics, Computer Science, Engineering, Physical Sciences, or a related field.
- Working knowledge of crystallographic data collection, processing, molecular modeling, and model validation.
- Expertise with modern object-oriented and version controlled software development.
- Proficiency with Linux, Python, and C++.
- Strong analytical skills including the ability to analyze complex problems, develop strategies to solve while running appropriate controls to validate accurate results.

- Demonstrated oral and written communication skills including a record of successful publications in recognized peer-reviewed journals.
- Excellent interpersonal skills including the experience effectively working in a collaborative R&D research environment as part of an interdisciplinary team.

What We Prefer:

- A Ph.D in Biophysics, Bioinformatics, Mathematics, Computer Science, Engineering, Physical Sciences, or a related field.
- Demonstrated excellence in signal processing, image processing, and multivariate statistics.
- Experience with GPU computing.
- Experience in a high-performance computing environment.
- Experience with Machine Learning (i.e. TensorFlow or PyTorch).

For full consideration, please apply by July 15, 2022 with the following application materials:

- Cover Letter - Describe your interest in this position and the relevance of your background.
- Curriculum Vitae (CV) or Resume.

Notes:

- This is a full time, exempt from overtime pay (monthly paid), 2 year (benefits eligible) Term appointment with the possibility of renewal up to a maximum of 5 years total based upon satisfactory job performance, continuing availability of funds, and ongoing operational needs.
- Salary is commensurate with experience.
- This position may be subject to a background check. Any convictions will be evaluated to determine if they directly relate to the responsibilities and requirements of the position. Having a conviction history will not automatically disqualify an applicant from being considered for employment.
- Work will be performed onsite at Lawrence Berkeley National Lab, 1 Cyclotron Road, Berkeley, CA.

How To Apply

Apply directly online at <http://50.73.55.13/counter.php?id=232201> and follow the on-line instructions to complete the application process.

Learn About Us:

Berkeley Lab (LBNL) addresses the world's most urgent scientific challenges by advancing sustainable energy, protecting human health, creating new materials, and revealing the origin and fate of the universe. Founded in 1931, Berkeley Lab's scientific expertise has been recognized with 13 Nobel prizes. The University of California manages Berkeley Lab for the U.S. Department of Energy's Office of Science.

Working at Berkeley Lab has many rewards including a competitive compensation program, excellent health and welfare programs, a retirement program that is second to none, and outstanding development opportunities. To view information about the many rewards that are offered at Berkeley Lab - Click Here (<https://benefits.lbl.gov/>).

Based on University of California Policy - SARS-CoV-2 (COVID-19) Vaccination Program and U.S Federal Government requirements, Berkeley Lab requires that all members of our community obtain the COVID-19 vaccine as soon as they are eligible. As a condition of employment at Berkeley Lab, all Covered Individuals must Participate in the COVID-19 Vaccination Program by providing

proof of Full Vaccination or submitting a request for Exception or Deferral.
Visit covid.lbl.gov (<http://covid.lbl.gov/>) for more information.

Berkeley Lab is committed to Inclusion, Diversity, Equity and Accountability (IDEA, <https://diversity.lbl.gov/ideaberkeleylab/>) and strives to continue building community with these shared values and commitments.

Berkeley Lab is an Equal Opportunity and Affirmative Action Employer. We heartily welcome applications from women, minorities, veterans, and all who would contribute to the Lab's mission of leading scientific discovery, inclusion, and professionalism. In support of our diverse global community, all qualified applicants will be considered for employment without regard to race, color, religion, sex, sexual orientation, gender identity, national origin, disability, age, or protected veteran status.

Equal Opportunity and IDEA Information Links:

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