

LCLS Call for Protein Crystal Screening Proposals

Closing Date: March 21, 2016

SUBMIT NEW PROPOSALS BY 4 pm PACIFIC on March 21, 2016 for Run 14 (Aug – Dec 2016)

The LCLS Protein Crystal Screening (PCS) program aims to enable increased access to LCLS beamtime for biological structure determination by making use of short, 6-hour runs to screen the quality of different sample preparations or potentially collect a full data set under good running conditions. To enable measurements within such a short time frame and maximize efficiency and the chances of success, these studies must be carried out with limited flexibility to minimize the time impact of setup changes. The following configurations are expected to be supported for PCS in this current call for proposals: gas dynamic virtual nozzle (GDVN) liquid jet system and fixed targets in vacuum at CXI. Other liquid jet systems supplied by user groups compatible with the basic CXI system will also be considered if the schedule allows it and at the discretion of LCLS. Furthermore, atmospheric pressure measurements on fixed targets using a goniometer system at MFX are expected to be available. Measurements using other demonstrated atmospheric pressure sample delivery techniques can be considered if the schedule allows it and at the discretion of LCLS. Schedule constraints are unpredictable and no guarantees can be made that any of the mentioned experimental setups will be available for PCS in any given run.

PCS at CXI

PCS experiments at CXI are intended to be carried out using the standard CXI configurations, either using the 1 μm or 100 nm focus depending on scheduling constraints. User-supplied sample delivery systems or modifications to the existing system can be allowable only if they are compatible with the existing systems and can be exchanged with the other systems used for PCS beamtime within a time frame compatible with 6-hour runs and rapid turnaround between groups. Decisions on using alternative sample delivery systems will be entirely at the discretion of LCLS.

PCS at MFX

PCS experiments at atmospheric pressure are expected to be available. The home of such experiments has moved from the XPP instrument to the MFX instrument, with a goniometer system allowing scanning of fixed-mounted crystals and for liquid jets of various kinds. These systems can also be modified in principle for use of a variety of atmospheric pressure sample delivery systems. The availability of all these systems will depend on scheduling constraints.

Other Experimental Geometries or Capabilities

Time-resolved studies and spectroscopy are currently not within the possible scope of PCS beam time.

Proposal Review and Beamtime Award

These PCS proposals will be reviewed by the PRP BIO-C panel separately from the regular proposals. It is desirable to shorten the period between PCS proposal submission and beam time allocation to maximize flexibility and the ability to be reactive to novel samples or ideas. LCLS will aim to pre-allocate blocks of beamtime either on CXI or MFX based on the overall demand. The expected amount of beamtime is on the order of 2 blocks of 10x6 hours shifts in every LCLS run. All PCS proposals will get a numerical rank from the BIO-C panel. A suitable number of proposals will be awarded beam time by LCLS based on the advice of the Proposal Review Panel. Successful proposals will be scheduled according to sample readiness and technical feasibility evaluation by LCLS staff scientists. A minimum 2 months notice will be given to the selected user groups to allow for appropriate preparation.

Overlap with Regular LCLS Proposals

There is no restriction with regards to possible overlap or redundancy with regular LCLS proposals. Submission of PCS proposals similar or related to regular LCLS proposals are encouraged and will not adversely impact the rankings of either types of proposals. Regular LCLS proposals that do not receive beamtime may be considered for PCS if deemed suitable.

Proposal Format

PCS proposals follow a similar format as regular proposals but must be submitted separately.

If the PCS proposal is related to one or more regular LCLS proposals that have been submitted or already received beam time, state this in the proposal.

LCLS PCS proposals should be submitted through the [User Portal](#).

Provide a descriptive title of your proposed experiment that you would be willing to be made public if awarded beam time.

PCS proposals are limited to a two-page PDF, including references, figures, and sufficient information to evaluate the impact, originality, need for LCLS, scientific risk, prior results, as well as technical feasibility. Pages should have at least 1 inch margins and not less than 10 pt font. The content should include:

- **Experimental Team:** In a table, list the names, institution, email address of PIs and collaborators who would participate in the proposed experiment (e.g., sample prep, theory, data collection, data analysis). This section could also briefly mention directly-relevant previous work done by the team members.
- **Scientific Case:** Briefly explain the background and significance of your experiment. In particular, why is LCLS required for this experiment? Itemize the specific aims and particular questions you want to answer. Focus on the specific experiment and avoid broad discussions in general terms.
- **Experimental Procedure:** Tell us if you plan or have carried out supporting experiments at other facilities. Have simulations of the experiment been performed? What are the anticipated data rates? Provide a beam time plan, indicating what could be accomplished in less than 6 hours of beam time. Describe any additional equipment you plan to bring to LCLS for the experiment. We strongly recommend

that you contact LCLS Scientist Mark Hunter (mhunter2@slac.stanford.edu) before proposal submission to discuss capabilities, to identify possible problems in integrating external equipment with the LCLS facility and to determine possible solutions.

- **Technical Feasibility:** Proposals must contain sufficient information for the LCLS to review the proposal for technical feasibility. This information should include:
 - Equipment
*Which elements of the proposed instrument do you require for the proposal?
What additional equipment is needed, detector, sample delivery/environment, temperature, pressure, etc.?
How do you plan to provide/organize the additional equipment?*
 - Parameters
Describe X-ray wavelength, pulse energy, bandwidth, beam size, repetition rate, pulse duration
 - Experimental protocol
*Describe the experimental geometry.
Calculate the expected signal rate/background.
Describe samples and concentrations, sample preparation and storage.
Describe local facilities that may be required.*

* Safety related documents must be submitted during the safety assessment portion of the LCLS proposal submission process in the user portal. List and describe any safety concerns that may arise with samples you will examine, equipment you will use, or techniques you will perform (including any physical, chemical or biological hazards) and how these issues will be addressed in the experiment design.

For more details of MFX, see:

https://portal.slac.stanford.edu/sites/lcls_public/Instruments/mfx/Pages/default.aspx

For more details of CXI, see:

https://portal.slac.stanford.edu/sites/lcls_public/instruments/cxi/Pages/default.aspx