# 9<sup>th</sup> Call for Proposals for User Experiments: Regular Proposals, Protein Crystal Screening Proposals, and, on invitation, Long-Term Proposals and Molecular Water Research Proposals



The 9<sup>th</sup> call for regular proposals at the European X-Ray Free-Electron Laser Facility (European XFEL) is open until **Wednesday**, **22 June 2022**, **at 16:00 (local Hamburg/Schenefeld time / Central European Summer Time – CEST)** for all six scientific instruments currently in operation. Please apply via the <u>User Portal to the European XFEL (UPEX)</u>.

- In the framework of this call, standard configurations for the HED, MID, and SCS instruments can be specified in the UPEX proposal form.
- A specific call for Protein Crystal Screening (PCS) proposals is also open at SPB/SFX, with the same deadline as the regular call.
- Spokespersons of selected Expressions of Interest in Long-Term Proposals and Molecular Water Research have been requested to submit their detailed proposals in specific calls on invitation, with the same deadline as regular/PCS proposals. Only invited proposals will be accepted in these calls.

Refer to the complete announcement below for other important information for all applicants.

A virtual information meeting will be held on Thursday, 12 May 2022 at 17:00 (local Hamburg/Schenefeld time / Central European Summer Time – CEST). Details about the videoconference link and agenda will be posted on our website soon.

Beamtime will be allocated from February to June 2023 at the following scientific instruments:

- Femtosecond X-Ray Experiments (FXE) at Beamline SASE1
- Single Particles, Clusters, and Biomolecules and Serial Femtosecond Crystallography (SPB/SFX) at Beamline SASE1
- High Energy Density Science (HED) at Beamline SASE2
- Materials Imaging and Dynamics (MID) at Beamline SASE2
- Spectroscopy and Coherent Scattering (SCS) at Beamline SASE3
- Small Quantum Systems (SQS) at Beamline SASE3

Instrument overview: https://www.xfel.eu/facility/instruments

Please check with the relevant instrument group about specific feasibility conditions for this call before submitting a proposal. Please also inquire with the instrument groups for more information about planned user community projects.

- **FXE**: christopher.milne@xfel.eu

- SPB/SFX: <a href="mailto:spb.sfx@xfel.eu">spb.sfx@xfel.eu</a>

- HED: ulf.zastrau@xfel.eu

- MID: mid-info@xfel.eu

- SCS: scs@xfel.eu

- SQS: michael.meyer@xfel.eu

All proposals submitted in this call will be reviewed for their scientific quality by panels of

international experts and checked for safety and feasibility conditions.

#### 1. Standard instrument configurations in this call

An efficiency advantage can be established on some instruments with the development of "standard configurations". The goal is to allow user experiments to be grouped together back-to-back without involving a major change in setup every time. In addition, these standard configurations will help provide a pathway to broaden the user community by reducing the need for user teams to include the expertise needed to design/construct and install specific endstation components. A range of standard configurations may be offered by an instrument, alternating throughout a period that covers several calls, to limit the range of required setups on a temporary basis. A number of instruments will make available standard configurations in this call.

## 1.1 HED standard configurations

### 1.1.1 Diamond Anvil Cell (DAC) standard configuration

- IC2 standard DAC setup, symmetric DAC cell support for users who need cells, user-supplied BX90 with adapters
- Optical observation microscope, streaked pyrometry for X-ray heating
- 18 keV SASE, max. rep. rate of 4.5 MHz, >0.5 mJ pulse energy from the undulators (not accounting for beamline transmission)
- 5–15 micrometer focal spot size (fixed at 5 μm, but effectively larger, depending on beam pointing stability)
- Detectors: AGIPD mini-half detector and VAREX flatpanel
- Required: Contact the HED instrument group for a feasibility check

#### 1.1.2 ReLaX-SAXS-PCI standard configuration.

- IC1 chamber, 100 TW ReLaX laser incident on target at 45° w. r. t. XFEL (no normal incidence of laser on target)
- SAXS+PCI @ 8.15 keV SASE (tunable within reasonable range), ca. 1 mJ per pulse, 2.25 MHz maximum rep. rate
- +5–50 µm spot size (both X-ray and ReLaX), no nanofocus possibility
- +PCI resolution of about 1µm
- Backward HAPG X-ray spectrometer, forward spectrometer can be added only if SAXS diagnostics is not used
- Laser diagnostics (upon request): EMP, electron, bremsstrahlung, and proton diagnostics
- Further details: Contact the <u>HED instrument group</u>

#### 1.2 MID – Small-angle MHz XPCS standard configuration

- AGIPD MHz area detector, 1 Mpx, 200 µm pixel size
- Photon energy: 7–12 keV, up to 2 mJ/pulse, up to 200 pulses/train, 10 trains/sec
- Min. correlation function lag time 440 ns, max. lag time 88 μs
- q-range (8 m sample–detector distance): ~7e-3 0.1 Ang-1 (small angle scattering)
- Beam size on sample: 1–10 μm with local optics, >30 μm with tunnel optics

- Standard mounts for sample in capillaries and scanning
- Mounting of user-supplied sample environments possible (contact <u>MID instrument</u> group before proposal submission)
- Further details: Contact the MID instrument group

## 1.3 SCS - CHEM-RIXS standard configuration

- Photon energy range: 0.5–1.4 keV, up to 1.1 MHz
- Combined resolving power up to 3000 (mono+spectrometer), up to 30 μJ pulse energy (monochromatic 1<sup>st</sup> order)
- 30–50 fs pulse duration (incl. pulse stretching mono)
- Linear and circular polarization (linear-ver., and circ pol. offered with basic functionality—inquire for details)
- Sample delivery: Single cylinder 20–50 μm liquid jet, solvents: water, ethanol or isopropanol
- RIXS spectrometer scattering angle: 125 deg
- Optical laser delivery: 800 nm (2 mJ @ 113 kHz, 0.2 mJ @ 1.1 MHz), SHG (400 nm), and THG (266 nm)
- Further details: Contact the SCS instrument group

# 2. Protein Crystal Screening at SPB/SFX

A specific call for protein crystal screening (PCS) is open at the SPB/SFX instrument that combines sample characterization and injection tests in the laboratories, followed by screening beamtime at the SPB/SFX instrument.

This call predominantly aims for protein crystals; however, can also include non-protein crystals or other diffracting protein samples if in accordance with the PCS standard parameters (see table below).

Nozzles and injection support will be provided by the Sample Environment and Characterization (SEC) group. This call exclusively addresses injection by gas dynamic virtual nozzles (GDVNs) and double-flow focusing nozzles (DFFNs).

For further information, please contact <u>Katerina Dörner (katerina.doerner@xfel.eu)</u> to submission.

#### Standard Parameters for PCS\*

Photon energy	9.3 keV
Detector distance	125 mm (approx. 1.7 Å edge resolution)
FWHM focus size	3.5 um
Sample delivery	Low viscosity liquid jet (GDVN, DFFN)

<sup>\*</sup> Minor changes to some of these parameters may occur due to logistics during the user run

PCS proposals, which are to be submitted to a specific call in the user portal UPEX, will be selected after peer review (including feasibility and safety checks).

### 3. Cross-instrument proposals

Highly targeted experiment proposals for a specific instrument have better chances of success. If, on the advice of our scientists, specific parts of your project should be conducted on different European XFEL instruments, the selection of two instruments is possible in the proposal form. Make sure that the proposal addresses the experiment

sessions on both instruments exhaustively. For schedule reasons, the proposal will receive individual IDs on submission and will be reviewed by both instrument proposal review panels concerned. This option should **not** be u

sed to submit the same experiment to two different instruments in order to increase the chances for beamtime allocation!

## 4. X-ray beam conditions for the allocation period

The conditions expected for this allocation period are listed below. **Nevertheless**, case-by-case verification of specific feasibility conditions with the instrument groups is required.

	Photon energy range	Expected pulse energy**
SA1	5–9.3 keV	2 mJ
	>9.3–14 keV	1 mJ
	>14-24 keV	0.5 mJ
SA2	5.8–9.3 keV	2 mJ
	>9.3–12 keV	1 mJ
	>12-24 keV	0.5 mJ
SA3	0.5–1.5 keV	5 mJ
	>1.5–2.5 keV	2 mJ
	>2.5 keV	0.5 mJ

Bunch distribution: 350 X-ray pulses per instrument assume equal distribution at 2.25 MHz operation. Higher or smaller numbers for higher/smaller intra-train frequency. Max. 2250 electron bunches within 500 µs are available for distribution to the instruments (4.5 MHz) \*\* Pulse energy depends on bunch charge, electron energy, and photon energy.

#### **Explanations:**

- 1. The above parameters correspond to the *standard* SASE operation mode.
- 2. The following *special* modes are available but require more tuning and are less reliable:
- a. Hard X-ray self-seeding (SA2; 7– 14 keV)
- b. Hard X-ray two-colour w. variable delay (SA2; 6–10 keV; 0–0.5 ps)
- c. Soft X-ray two-colour w. variable delay (SA3; 500-3000 eV; 0-1 ps)
- d. Short bunches (< 10 fs FWHM); requires coordinated scheduling, as other instruments and available number of bunches might be affected; time-diagnostics is only partially available
- e. Full trains at instruments with << 10 Hz rep. rates (~ 2250 pulses)

Experiments requesting these *special* modes should address the development of new techniques and fields and are expected to involve large communities and facility staff. If included in the final schedule, continuous (24 hr) beam delivery would be planned in this case. Since there is a vast range of detailed specifications for these special modes, proposers are requested to contact the corresponding instrument staff in order to clarify requirements.

## 5. Experiment reports about previous beamtime

Experiment reports are mandatory and must be submitted 3 to 6 months after the end of each experiment. However, Main Proposers and/or Principal Investigators who have received beamtime in the past and who submit new proposals or continuation proposals must provide the experiment reports related to previous proposal(s) via the User Portal to the European XFEL (UPEX) by Friday 24 June 2022. Missing experiment reports may result in withdrawal of new proposals from the review process. Please refer to further instructions on our homepage.

## 6. Operation during COVID-19 pandemic

At present, it cannot be excluded that the travel restrictions that affected previous user runs and the <u>specific hygiene measures applying to user operation at our facility</u> this year will also influence operational aspects in the first part of 2023.

In the proposal form, you are requested to detail to what degree your proposal would be affected by the persistence of pandemic conditions and what measures could be taken in order to mitigate these consequences, still preserving good chances of success.

In case of doubt, please contact the instrument groups for advice.

### 7. User pages and funding options

More practical information for users can be found here:

https://www.xfel.eu/users

**Travel funding** and living subsistence are available for a number of users affiliated with organizations based in the member countries of European XFEL.

Further details are available here:

https://www.xfel.eu/users/user\_guide/funded\_user\_travel

Specific **shipping funding options** for organizations based in the member countries of European XFEL are available in order to mitigate the impact of COVID-19 travel restrictions.

European XFEL User Office Email: <a href="mailto:useroffice@xfel.eu">useroffice@xfel.eu</a>

Phone: +49 (0)40 8998-6937 or -6767

Please always check with the relevant instrument group about specific feasibility conditions before submitting a proposal.

- **FXE**: <u>christopher.milne@xfel.eu</u>

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- SQS: michael.meyer@xfel.eu