# 11<sup>th</sup> Call for Proposals for User Experiments: Regular Proposals (including Cross-Instrument Use) and Sample and Protein Crystal Screening Proposals



The 11<sup>th</sup> call for proposals at the European X-Ray Free-Electron Laser Facility (European XFEL) is open until **Thursday**, **11 May 2023**, **at 16:00 (local Hamburg/Schenefeld time / Central European Summer Time – CEST)** for the seven scientific instruments in operation in the first semester of 2024. Please refer to the important information below and apply via the <u>User Portal</u> to the European XFEL (UPEX).

- In the framework of this call, the choice of a **standard configuration for the HED and the MID instruments** (see Section 1. below) must be specified in the UPEX proposal form. At HED, priority access for the HIBEF User Consortium will reduce the available general user time by 30%. Questions regarding priority access should be directed to the HIBEF User Consortium spokesperson Prof. Thomas Cowan (HZDR) (contact information on the HIBEF webpage).
- Note that, the SXP instrument will only accept proposals for the standard configuration described in section 1.3 below.
- The SCS instrument only accepts proposals for solid samples using the FFT station in forward-scattering geometries and for the CHEM station providing liquid jet sample environments. Details can be found in the fact sheet on the SCS instrument site. In order to support experiment proposals from the chemistry RIXS community, the lower photon energy range at SASE3 will be adapted in this allocation period, so as to include the N K-edge at 410eV.
- A specific call for Sample and Protein Crystal Screening (PCS) proposals is also open at SPB/SFX with the same deadline as the regular call.

A virtual information meeting will be held on Thursday, 20 April 2023 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 2024 (run 2024-I) at these 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
- Soft X-Ray Port (SXP) at Beamline SASE3

Instrument overview: <a href="https://www.xfel.eu/facility/instruments">https://www.xfel.eu/facility/instruments</a>

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

- SXP: sxp@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 end station 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. Access to the SXP instrument in this run is only possible in the standard configuration described in section 1.3 below.

#### 1.1 HED standard configurations

**Statement about alternating setups:** DiPOLE and DAC proposals compete for the same resources, e.g. beamtime at 16.3 GeV electron energy and IC2 target chamber access. Therefore, European XFEL decided to only schedule the DiPOLE platform in 2023-II, and consequently in call 11 for 2024-I, no DiPOLE proposals will be accepted, in favor of DAC proposals and minimum setup change-overs. We anticipate that in the next call 12 (opening in the second half of 2023), no DAC proposals will be accepted in favor of DiPOLE proposals

#### 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>

## 1.1.3 DiPOLE 100-X standard configuration

• not available for in this call (see above). DiPOLE will be available again in call 12.

# 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<sup>-1</sup> (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 group</u> before proposal submission)
- Further details: Contact the MID instrument group

## 1.3 SXP – Time-resolved photoelectron spectroscopy standard configuration

- Spatial and momentum resolved k-microscope photoelectron spectrometer equipped with a delay-line detector.
- Photon energy: > 0.5 -- 3 keV, > 200 pulses/train, 10 trains/sec
- Beam size on sample: 3 500 μm, default ~30 μm
- Omicron type mount for solid samples
- Load lock for fast sample insertion and preparation chamber
- Further details: Contact the SXP instrument group

#### 2. Sample and Protein Crystal Screening at SPB/SFX

A specific call for Sample and 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, non-protein crystals or other diffracting protein samples are welcome 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 screening call exclusively addresses injection by gas dynamic virtual nozzles (GDVNs) and double-flow focusing nozzles (DFFNs). For further information, please contact Katerina Dörner (katerina.doerner@xfel.eu) prior to

#### Standard Parameters for PCS\*

submission.

Photon energy	9.3 keV
Detector distance	125 mm (approx. 1.7 Å edge resolution)
FWHM focus size**	0.3 µm or < 200 nm
Sample delivery	Low viscosity liquid jet (GDVN, DFFN)

<sup>\*</sup> Minor changes to some of these parameters may occur

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). More details are available on the SPB/SFX web page.

<sup>\*\*</sup> Use of the micro or nano focus will be determined based on the standard configuration for the scheduling of the user run

# 3. Cross-instrument proposals

If, <u>on the advice of our scientists</u>, specific parts of your project should be conducted by using different European XFEL instruments, the selection of two instruments is allowed in the proposal form in order to submit a cross-instrument proposal. Make sure that the proposal addresses the experiment sessions on both instruments exhaustively.

For schedule reasons, the cross-instrument proposal will receive individual IDs on submission and will be reviewed by both instrument proposal review panels concerned. *This option should not be used to submit the same experiment to two different instruments in order to increase the chances for beamtime allocation.* Highly targeted experiment proposals for a specific instrument have better chances of success.

### 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**
	5–9.3 keV	2 mJ
SA1	>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
	0.4–1.5 keV	5 mJ
SA3	>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  $\mu s$  are available for distribution to the instruments (4.5 MHz). Exact bunch distribution is based on needs of particular experiments and the capabilities of the photon delivery systems.

\*\* 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 may require more tuning and could be 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; 400–3000 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.

Figure 1 shows the general relation between photon energy and electron energy.

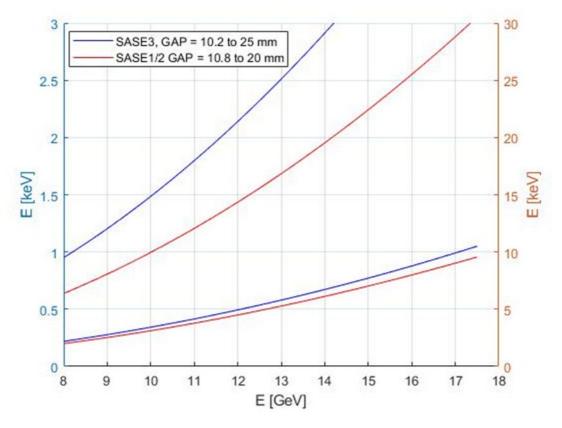


Figure 1) Maximum and minimum reachable photon energies for SASE1/2 (red) and SASE3 (blue) versus Electron Energy.

#### 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 Monday 15 May 2023. Missing experiment reports may result in withdrawal of new proposals from the review process. Please refer to the complete information on this web page.

# 6. Information for users and funding options

More practical information for users can be found here: https://www.xfel.eu/users/index\_eng.html

**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.

European XFEL User Office Email: <u>useroffice@xfel.eu</u>

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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MID: mid-info@xfel.eu

- SCS: scs@xfel.eu

- **SQS**: michael.meyer@xfel.eu

- SXP: sxp@xfel.eu