# 13<sup>th</sup> Call for Proposals for User Experiments: Regular, Screening and Molecular Water Research Proposals

The 13<sup>th</sup> call for proposals at the European X-Ray Free-Electron Laser Facility (European XFEL) is open until

#### Tuesday 30 April 2024, at 16:00 CEST

(local Hamburg/Schenefeld time / Central European Summer Time) for six of the scientific instruments. Please refer to the important information below and apply via the <u>User Portal to the European XFEL (UPEX)</u>. Beamtime will be allocated in the first semester of 2025 (run 2025-I) at these scientific instruments:

- Femtosecond X-Ray Experiments (FXE) at Beamline SASE1
- <u>Single Particles, Clusters, and Biomolecules and Serial Femtosecond</u> <u>Crystallography (SPB/SFX)</u> 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

Note that due to important maintenance tasks, European XFEL will not accommodate user experiments in the second semester of 2025. The next regular call for proposals after this current one will open in 2025, for experiments in 2026-I.

# Please check with the relevant instrument group about feasibility conditions for this call before submitting a proposal and for more information about user community projects.

- FXE: christopher.milne@xfel.eu
- SPB/SFX: spb.sfx@xfel.eu
- HED: ulf.zastrau@xfel.eu
- MID: mid-info@xfel.eu
- SCS: scs@xfel.eu
- SQS: michael.meyer@xfel.eu
- Within this regular call, the European X-Ray Free-Electron Laser Facility (European XFEL) would like to open a second call for proposals for User Experiments on Molecular Water Science in the allocation period 2025-I. Following on the steps of our first successful call, an average of one beamtime slot per instrument has been reserved for successful proposals. This call shall cover an extended scope and we accept also proposals on water solutions, energy/water splitting, environmental and climate research. Collaborations (joint proposals) between expert groups and newcomers are encouraged.
- 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.
- In the framework of this call and in addition to regular proposals, the option of standard configurations for the HED and the MID instruments (see Section 1. below) is available. The choice 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 spokesperson, Prof. Thomas Cowan (HZDR) (cf. <u>HIBEF webpage</u>).
- 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 <u>SCS instrument site</u>.
- **FXE** encourages users to take advantage of the demonstrated ability to perform solutionphase X-ray absorption spectroscopy (XAS) and wide-angle X-ray scattering (WAXS) at high photon energies (15-19 keV) at this instrument.



For this call, no virtual information meeting is planned. **Individual contact to the instrument** groups is strongly encouraged to discuss specific requirements and technical feasibility of proposals in detail.

For questions about status and plans at the facility, feel free to contact:

- <u>Serguei Molodsov</u> (Scientific Director for Soft X-Ray Experiments and Sample Environment and Characterization),
- <u>Sakura Pascarelli</u>: (Scientific Director for Hard X-Ray Experiments)

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-toback 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.

# 1.1 HED standard configurations

HED users are always welcome to submit regular (non-standard platform) proposals which fit to the instrument capabilities, according to the details given in the pdf document linked to our HED-HIBEF website. However, before submitting, it is mandatory to discuss your proposal with the instrument staff, as not all combinations of our capabilities are technically feasible.

**Statement about alternating setups:** DiPOLE XRD and DAC XRD 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 schedule the DiPOLE XRD IC2 platform in each second half of a calendar year. Consequently, in this call for 2025-I, no standard DiPOLE IC2 XRD proposals will be accepted, in favour of DAC XRD proposals and minimum setup change-overs. We anticipate that in the next call 14 (in Spring 2025 for allocation in run 2026-I), no DAC XRD proposals will be accepted in favour of DiPOLE IC2 XRD proposals. Please note that this scheme does not apply to DiPOLE spectroscopy proposals at lower photon energies for IC1. The following standard configurations will be available in the allocation period related to this call:

# 1.1.1 ReLaX-SAXS-PCI standard configuration

Details: Conditions for the 13<sup>th</sup> call for proposals are on the HED web pages <u>https://www.xfel.eu/facility/instruments/hed/documentation/index\_eng.html</u> The <u>HED instrument group</u> is available for questions and discussion of your project.

# 1.1.2 Diamond Anvil Cell (DAC) standard configuration

Details: Conditions for the 13<sup>th</sup> call for proposals are on the HED web pages <u>https://www.xfel.eu/facility/instruments/hed/documentation/index\_eng.html</u> The <u>HED instrument group</u> is available for questions and discussion of your project.

### 1.1.3 DiPOLE 100-X standard configuration

This configuration is <u>not available</u> in this call (see above) and will be offered again in call14 opening in Spring 2025 / allocation period 2026-I.

# **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 SCS configurations in this call

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 <u>SCS instrument site</u>.

In order to support experiment proposals from the chemistry RIXS community, the lower photon energy range at SASE3 will include the N K-edge at 410eV.

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

In addition to the regular call for proposals which can take advantage of the full instrument capability detailed on the <u>SPB/SFX website</u>, 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 <u>Katerina Dörner (katerina.doerner@xfel.eu)</u> prior to submission.

#### Standard Parameters for PCS\*

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)

\* Minor changes to some of these parameters may occur \*\* Use of the micro or nano focus will be determined based on the standard configuration for the scheduling of 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). More details are available on the <u>SPB/SFX web page</u>.

# 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 and the experiment description addresses experiment sessions on both instruments exhaustively. For schedule reasons, the cross-instrument proposal will receive individual IDs on submission to both instruments 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. New for the allocation period 2025-I is the provision of variable polarization radiation at the SASE3 FEL and the provision of attosecond pulses at SASE3. Both of these modes are included for the first time in the call for user experiments, However, at present very few experiences have been collected and, in addition, a wide range of possible parameters could be selected. Both modes are still under development and we therefore consider them as special modes. For specific parameters (photon energies, polarization states, purity, expected pulse durations), you need to inquire with the respective instruments.

# 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
	5.8–9.3 keV	2 mJ
SA2	>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. The values in this table refer to average pulse energies in an optimized parameter setting. Depending on how much the actual parameters differ from these optimum values, the attainable pulse energies can be lower. It is very important to contact the instruments in order to evaluate the feasibility of your requirements

#### Explanations:

- 1. The above parameters correspond to the *standard* SASE operation mode.
- 2. The following *non-standard* 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)
  - 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)
- 3. The following *special* modes are available but will likely require more tuning and may be less reliable. Interested PIs are strongly encouraged to contact the Leading Scientist of the respective instrument prior to proposal submission.
  - a. Variable polarization (circular left/right; linear) at SASE3 (so far tested 700 900 eV)
  - b. Attosecond pulse delivery at SASE3 (e.g. ≥200 as, few 100 µJ @ 1 keV)

Experiments requesting these *non-standard* and *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 h) 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 Monday 06 May 2024. Missing experiment reports may result in withdrawal of new proposals from the review process. Please refer to the complete information on this web page:

https://www.xfel.eu/users/user\_guide/experiment\_report/index\_eng.html

#### 6. Information for users and funding options

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

• **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:
  <u>https://www.xfel.eu/users/user\_guide/funded\_user\_travel</u>
- Specific **shipping funding options** for organizations based in the member countries of European XFEL are available: https://www.xfel.eu/users/user\_guide/shipping/index\_eng.html
- General enquiries can be directed to the European XFEL User Office Email: <u>useroffice@xfel.eu</u> Phone: +49 (0)40 8998-6937 or -6767

# Before submitting a proposal, always check with the relevant instrument group about specific feasibility conditions

- FXE : <u>christopher.milne@xfel.eu</u>
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- SCS : <u>scs@xfel.eu</u>
- SQS : michael.meyer@xfel.eu