TECHNICAL NOTE

UPEX: Experiment Proposal and Registration Guide

October 2021

S. Bertini
for the User Office
at the European XFEL



Germany

Revisions

Version	Date	Description	
3.0	21 Oct. 2021	 Updated preface to reflect evolutions in the database allowing to enter and save symbols and special characters in proposal fields Added Section 1.1.3, "Mailing lists" Added Section 2.2.5, "Sample coordinator" Added Section 2.3.1, "Choice of scientific instrument" Added Section 2.3.2, "Cross-instrument proposals" Added Section 2.3.7, "Standard instrument configurations" Added Section 2.3.8, "Choice between standard and custom instrument configurations / beam properties" Added Sections 2.4, "Special proposals" Added Section 2.4.1, "Protein Crystal Screening (PCS) proposals" Updated Chapter 3, "Registering for experiments in UPEX" Updated Section 4, "Feedback" Updated Appendix B, "Useful email contacts" 	
2.5	28 May 2019	 Updated Section 1.2, "UPEX lightweight account vs. Campus account" Added Section 2.3.4.5, "Proposal continuation or resubmission" 	
2.4	14 May 219	 Updated preface Updated Section 1.2, "UPEX lightweight account vs. Campus account" Updated Section 2.3.4.1, "General information" Updated Section 2.3.4.6, "Abstract" Updated Section 2.3.4.7, "Description of Proposed Experiment" Updates Section 2.3.9, "Resources and Additional Instrumentation" 	
2.3	29 Nov. 2018	 Updated Section 2.2, "Attribution of responsibilities within the user team" Updated Section 2.3.4.4, "Instrument team contacted" Updated Section 2.3.6, "Beam properties and instrument configuration" Updated Section Error! Reference source not found., "Error! Reference source not found.", including new Section Error! Reference source not found." 	
2.2	11 May 2018	■ Added new fields in Section 2.3, "European XFEL proposal form"	
2.1	18 Apr. 2018	 Updated Section 1.2, "UPEX lightweight account vs. Campus account" Added Chapter 4, "Feedback" 	
2.0	6 Oct. 2017	 Added information on Campus account vs. UPEX account Added new fields in proposal form Oct 2017 Added Chapter 3, "Registering for experiments in UPEX" 	
1.5	7 Apr. 2017	Added new log-on screen, new username, and recovery procedure	
1.4	23 Feb. 2017	Username character restrictions	
1.3	11 Jan. 2017	Sample/substance policy	
1.2	22 Dec. 2016	Various updates, sample/substance sheet update	
1.1	13 Dec. 2016	Procedure for personal profile changes, email verification, attribution of functions within user team	
1.0	14 Nov. 2016	First draft	

October 2021

2 of 43

XFEL.EU TN-2017-001-3.0

Contents

Revi	Revisions			2
Prefa	ice			5
1	Regi	stering i	n UPEX	7
	1.1	How to	register	7
		1.1.1	Registration rules	
		1.1.2	Email verification	
		1.1.3	Mailing lists	9
	1.2	UPEX I	ightweight account vs. Campus account	
		1.2.1	Changing passwords for Campus or UPEX lightweight accounts	
		1.2.2	Recovering passwords for Campus or UPEX lightweight	
			accounts	11
	1.3	Log-on	screen	11
	1.4	Your U	PEX homepage	12
		1.4.1	Edit profile	13
		1.4.2	Proposals	
	1.5	Icons u	sed in UPEX	15
2	Subr	nitting p	roposals	16
	2.1	Genera	l rules	16
	2.2	Attributi	on of responsibilities within the user team	17
		2.2.1	Principal Investigator	18
		2.2.2	Main Proposer	18
		2.2.3	Proposers	18
		2.2.4	Participants in the experiment	18
		2.2.5	Sample coordinator	18
	2.3	Europe	an XFEL proposal form	19
		2.3.1	Choice of scientific instrument	19
		2.3.2	Cross-instrument proposals	19
		2.3.3	Navigation	20
		2.3.4	General part	20
		2.3.5	Sample/Substance Sheets	24
		2.3.6	Beam properties and instrument configuration	26
		2.3.7	Standard instrument configurations	26
		2.3.8	Choice between standard and custom instrument	
			configurations / beam properties	
		2.3.9	Resources and Additional Instrumentation	29
		2.3.10	Laboratory access	32
	2.4	-	proposals	
		2.4.1	Protein Crystal Screening (PCS) proposals	33

3	Reg	Registering for experiments in UPEX		
	3.1 Registration of Experiment Team (A-form) and Personal Arrival F			
		(PAF) .		35
		3.1.1	A-form (Arrival Form)	35
		3.1.2	Personal Arrival Form (PAF)	37
		3.1.3	Lab access requests	38
	3.2	Attribution of responsibilities within the user team		38
		3.2.1	Principal Investigator	38
		3.2.2	Main Proposer	38
		3.2.3	Co-Proposers	
		3.2.4	Participants in the experiment	39
4	Feed	dback		40
	4.1 Experiment reports .		ment reports	40
		4.1.1	General rules for experiment reports	
		4.1.2	Instructions for uploading your experiment report to UPEX.	41
	4.2	4.2 Feedback form		
Α	Ack	nowledg	ements	42
В	Useful email contacts			43

Preface

The European XFEL (EuXFEL) is a research facility open to scientists worldwide. Beamtime is free of charge, but experiment proposals must go through a review process. Proposal must be submitted through the User Portal to the European XFEL (UPEX). As an important condition for access, after the experiments, the authors must strive to publish the results in peer-reviewed journals.

Before you start using UPEX, please be aware of some basic features depending on database criteria:

- Fields in the registration and proposal form should be completed in English. Names should be transcribed into standard Latin characters.
- Please be aware that symbols may not be saved if imported into a form field¹. In this case, we recommend a transcription into Latin script (e.g. α = alpha, β = beta). However, since an upgrade to the database in summer 2020, a larger number of symbols can be saved when entered in a form field. However, please note that text entries in proposals submitted before this upgrade will not benefit from the same possibility. CHANGES IN THE PROPOSAL FORM: In the framework of the CALIPSOplus EU project, in order to offer a better service to users, all European synchrotrons and free-electron lasers (FELs) have agreed upon a common list of proposal form labels. Therefore, some labels in the European XFEL proposal form in UPEX had to be changed with respect to the past calls. You will find more information about his under: http://www.wayforlight.eu/en/users/spf/

XFEL.EU TN-2017-001-3.0

¹ Following the ISO/IEC 8859-1 Standard.

In particular, in May 2019 the EXPERIMENT DESCRIPTION template (see your UPEX normal user dashboard) was amended to reflect this standardization.

Registering in UPEX

At the present stage, prospective users need a valid account in UPEX to be involved in any of the following tasks:

- Submitting a proposal (Main Proposer)
- Appearing on a proposal as Principal Investigator or Co-Proposer
- Reviewing proposals as a member of a PRP or as an external referee
- After a proposal has been allocated beamtime, being assigned to the experiment as a member of the user team (in case there is no perfect match with the list of proposers)

These different tasks are possible in the normal user role. This implies that none of the above is possible if registration in UPEX has not been correctly completed at a previous stage. Please allow for some time for processing in case your affiliation is not yet in our database and needs to be added by the EuXFEL User Office. In the future, more access functionality may be included.

1.1 How to register

To register in UPEX, follow these steps.

- From the EuXFEL website, and click on the link to UPEX: https://in.xfel.eu/upex
- 2 At the bottom of the UPEX log-on page, click Create New Account to open the registration form.
- **3** Fill in all fields, as requested.

Fields marked with an asterisk (*) are mandatory.

1.1.1 **Registration rules**

When registering in UPEX, follow these rules:

Username

Usernames can have only 4 to 8 lower-case alphabetic characters (a–z). They are case-sensitive and must be unique.

Password

Passwords are case-sensitive and must have at least 6 characters.

Email address

An existing unique email address is required to register. All correspondence relevant to the project and other important information will be sent to the email address you indicate. Please make sure you enter this information correctly.

Position

When attributing the Principal Investigator responsibility in your proposal, make sure that the relevant UPEX user has a staff position and that this information is stated in the appropriate field.

Affiliation

Select an affiliation from the existing database by clicking Select My Institute and searching by the name of the organization (mostly full name, abbreviation, or both) or town. If you do not find your affiliation, or if the name, address, or department is not correct, click the appropriate link at the bottom of the form to request support from EuXFEL User Office by email and give the correct information.

The same applies if your department is not listed for an organization that is already in our database.

1.1.2 **Email verification**

After you have registered, a validation email is sent to your email address.

CAUTION: This does not apply to EuXFEL or DESY staff.

To validate your email, click the validation link in the body of the message. Before you do this, make sure that the complete validation link is fully marked as such. If it is not, you can copy and paste the link in the body of the validation email into the location bar of your browser.



CAUTION: The validation must be completed within 24 hours from the time of registration. Failure to complete the validation in this timeframe will result in removal of the account.

1.1.3 Mailing lists

On registration to UPEX, you can subscribe to a number of mailing lists on specific topics related to our facility. Once you have a UPEX account, you can manage these mailing list subscriptions directly from your normal user profile.

Figure 1: Mailing list registration selection on registration

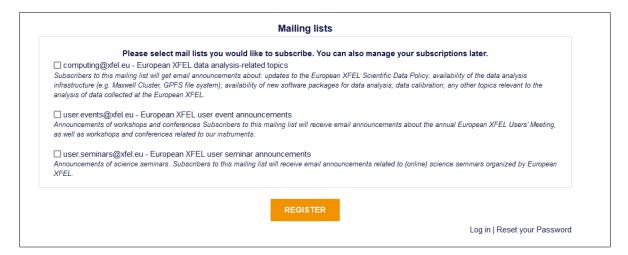
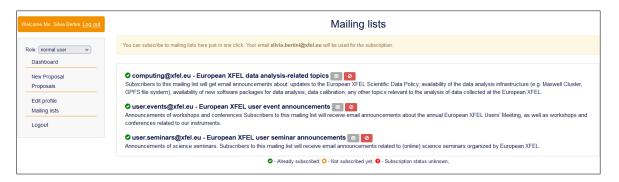


Figure 2: Managing mailing list subscriptions from the UPEX user profile



XFEL.EU TN-2017-001-3.0

1.2 **UPEX lightweight account vs. Campus** account

During your registration to UPEX (User Portal to the European XFEL), a lightweight account will be created for you. This account will not provide access to any other service but UPEX.

If your proposal is awarded beamtime, you will need to access other resources, services, software, and infrastructure, such as safety training, the experiment data access and processing system, different support resources, and so on. For this purpose, a Campus account will be set up for you (if you do not have it already) for accessing DESY/EuXFEL campus infrastructure and services. In due time, you will receive a notification email with your Campus account credentials and further instructions.

Please note:

- Campus accounts set up via UPEX lightweight accounts are provided and managed by the DESY registry. For the time being, you will get password expiration notifications from the DESY registry. However, password change or recovery takes place through UPEX. Please refer to the instructions below.
- You can create your Campus account password by clicking the link specified in the notification email (see above). Propagation of the new password to all of the services may take up to one hour.
- More details will be provided in the notification email, as already mentioned. Please DO NOT ignore it.

With your Campus account you will be able to access the online safety training system, metadata catalogue, and other services. We strongly recommend using your Campus account to log on to UPEX. Nevertheless, you may still use your lightweight account credentials for UPEX only (for example, if you need to access UPEX urgently before a deadline but do not remember your Campus credentials).

October 2021 XFEL.EU TN-2017-001-3.0 **10** of **43 UPEX: Experiment Proposal and Registration Guide** Users with an existing DESY/EuXFEL Campus account (e.g. DESY or EuXFEL staff members) are advised to use these credentials for logging on to UPEX and DESY/EuXFEL Campus services. If these users create a lightweight account in UPEX first, the relevant DESY/EuXFEL Campus account will be automatically associated with the lightweight one and can be used from this moment.

1.2.1 Changing passwords for Campus or UPEX lightweight accounts

The passwords for both your UPEX lightweight account and your Campus account can be changed from your Edit profile page after logging on to UPEX:

https://in.xfel.eu/upex/user/edit_profile?role=1

1.2.2 Recovering passwords for Campus or UPEX lightweight accounts

For any UPEX lightweight accounts and any Campus accounts *created by EuXFEL via the UPEX account*, the password can be reset from the UPEX password recovery page:

https://in.xfel.eu/upex/password/request_reset

If you forgot your EuXFEL/DESY Registry staff password, contact the IT administration of the organization to which you belong.

1.3 Log-on screen

Figure 3 shows the log-on screen of UPEX.

At the top of the log-on screen, you have the option to authenticate by using specific UPEX account credentials or EuXFEL/DESY credentials.

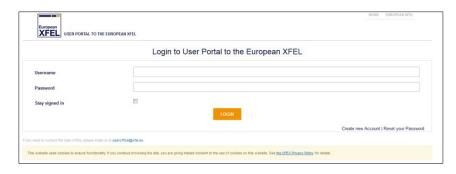
Authentication through an UMBRELLA account will be available at a later stage.

If you already have an account in UPEX, enter your username and password to log on to the system.

XFEL.EU TN-2017-001-3.0

October 2021

Figure 3: UPEX log-on screen



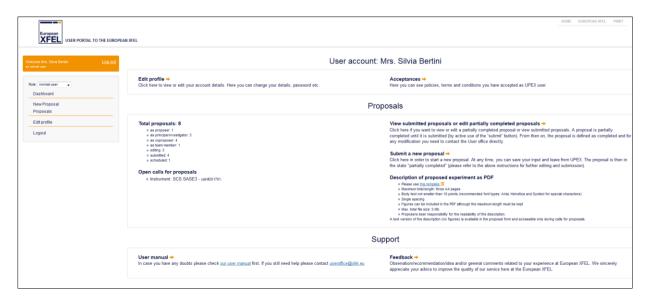
If you do not remember your password, you can click Reset Your Password, enter your username or the email address you listed when registering your account in UPEX, and confirm Reset Your Password. A password reset link will be sent to the email address (see Section 1.1.1, "Registration rules"). Open the email and click the reset link. You will be then re-directed to UPEX. Enter and confirm your new password in the form displayed. From there you will be able to log on directly. The new password will be active for all subsequent log-ons.

NOTE: If you do not remember your username, request a reset link by indicating your email address. The username will be indicated in the form displayed in UPEX after clicking the reset link. Otherwise, contact the EuXFEL User Office (useroffice@xfel.eu).

1.4 Your UPEX homepage

When you register for UPEX, the Normal User role is assigned by default, as shown in Figure 4.

Figure 4: Normal User dashboard in UPEX



1.4.1 Edit profile

If you select the Edit Profile option, you can update your personal details (e.g. including password, affiliation, and other contact information. After registration, it is possible to update this information without limitation. However, after a first change of your personal details, you be allowed to change them again only after 7 days.

1.4.2 Proposals

You can also access all of the functions described below through the left sidebar on your dashboard. If more than one UPEX role has been assigned to you, you can switch to the relevant dashboard (and the relevant options) from the dropdown list at the top of the left sidebar.

1.4.2.1 View or edit a partially completed proposal or view submitted proposals
By clicking the link View or Edit Partially Completed Proposals, you can view some information about the number of proposals in which you are involved.

A proposal is "partially completed" until it is actively submitted (by clicking the Submit button). From then on, you will not be able to change anything in the proposal.

By selecting the link, you can access an overview of the proposals you are involved in as Main Proposer, Principal Investigator (PI), or Co-Proposer, as shown in Figure 5. You can also view or download them as a PDF. Main Proposers also have the permission to edit partially completed proposals (i.e. proposals in Editing status) and submit them before the call deadline.

XFEL USER PORTAL TO THE EUROPEAN XFEL Proposals ld ↓ Title 2095 test 2 Markus Scholz SCS SASE3 6 Submitted 2017-09-26 08:15:34 Markus Scholz Ø⊕± Edit profile 2094 Test proposal WM Dr. Wolfgang Morgenroth Mrs. Silvia Bertini SCS SASE3 8 Submitted 2092 test 1 Markus Scholz Markus Scholz SCS SASE3 5 Submitted ©⊕± 2090 test for Sample sheet Mrs. Silvia Bertini Mrs. Silvia Bertini SCS SASE3* 5 Editing Ø⊕± 2089 Test Proposal with new UPEX Ms. Giulia Quondam Ms. Giulia Quondam SCS SASE3 5 Submitted Ms. Giulia Quondam Ms. Giulia Quondam MID SASE2 2017-04-19 🖸 🛈 🕹

Figure 5: Overview of proposals entered in UPEX as Main Proposer or Co-Proposer

1.4.2.2 Proposal withdrawal

To withdraw a submitted proposal, contact the EuXFEL User Office (<u>useroffice@xfel.eu</u>).

1.4.2.3 Submit a new proposal

Clicking Submit a New Proposal enables you to start the process of submitting a new proposal by opening the EuXFEL Proposal Form (PF).

1.5 Icons used in UPEX

In the UPEX graphical user interface (GUI), you can hover your mouse over any icon to get context-sensitive help. Clicking the icon executes the action.

Table 1: Definitions of UPEX icons

Icon	Name	Action
0	View	View a proposal in the UPEX GUI.
₹	Download	Download the PDF file of a proposal in which you are Main Proposer, PI or Co-Proposer at any stage.
Ø	Edit (green)	Edit the document/section of a form
Ø	Edit (grey)	Editing function is not available. For example, if this icon appears in the proposal overview on your dashboard, either you are not the Main Proposer who initiated submission and you do not have the corresponding privileges or the proposal was already submitted. For details, see Section 2.1, "General rules".
	Delete	Delete a specific form section.
,	Clone	Clone the current section (e.g. a sample sheet) and edit the copy to produce a new section.
*	Team coordinator (grey)	Main Proposer or other user team member who is attributed team coordination responsibility.
æ	Select new team coordinator (green)	Select a new team coordinator among the members of the team (e.g. if the Main Proposer will not attend the experiment).
Д	Sample coordinator	Select a sample coordinator within the team—this designation can be changed at the A-form step.

2 Submitting proposals

Over the first calls for proposals, our facility and the scope of operation will gradually develop. Updates on the status of the facility can be found on our website (www.xfel.eu). Information on instruments available to users is found in each specific call for proposals. If you need further information and support, contact the scientific teams of the instruments you are interested in or the EuXFEL User Office well before submitting your proposal. Useful contacts are provided in Appendix B, "Useful email contacts".

2.1 General rules

When submitting proposals, follow these important rules:

- To submit a proposal for beamtime at EuXFEL or be added as Co-proposer or Principal Investigator to the proposal, you must have a UPEX account.
- Submission is possible only <u>before</u> the deadline specified in the relevant call. After the deadline, it is <u>not</u> possible to submit proposals.
- Only complete proposals are accepted.
- Editing of not-yet-submitted proposals is possible only by the main proposer.
- It is <u>not</u> possible to save a page of the Proposal Form (PF) that contains incomplete mandatory fields.
- After submission, you will <u>not</u> be able to change a proposal by yourself.
- Information requested in the fields marked with an asterisk (*) is mandatory

- The experiment description is mandatory (see Section 2.3.4.7, "Description of Proposed Experiment").
- Submission of the experiment report for standard experiments is required between 3 to 6 months after end of last shift of the experiment at the latest. However, in the event of new proposals or continuation proposals by the same scientists (as Main Proposers and/or Principal Investigators), you must submit experiment reports via the User Portal to the European XFEL about all previous measurement(s) by the deadline for experiment reports indicated in the relevant call for proposals, including
 - Those carried out close to the proposal submission deadline
 - Experiments whose scientific area or instrument is different from those relevant to your new proposal
- Provide a reference to this experiment in your new proposal, by indicating the corresponding previous experiment ID in the field "Continuation / Resubmission" in the General part of the proposal form in UPEX.

2.2 Attribution of responsibilities within the user team

Please note that the attribution of functions in the proposal submission and allocation process within the user team has to be done through the selection of the relevant scientist at the proposal stage. Each scientist mentioned in a proposal with the role of Principal Investigator, Main Proposer, or Proposer receives an email confirmation from UPEX on proposal submission.

Main Proposers/Principal Investigators must seek the approval of all scientists they wish to add to the list of co-proposers of the proposal BEFORE proposal submission.

XFEL.EU TN-2017-001-3.0

In case you think that your name has been added in error to a proposal, please contact the EuXFEL User Office as soon as possible after receiving the automatic notification from UPEX.

2.2.1 Principal Investigator

Besides being in most cases the lead researcher or one of the lead researchers of the project addressed in the proposal, for the purpose of access to the EuXFEL facility, the Principal Investigator is specifically identified among the authors of the proposal and bears exclusive long-term responsibility for experiment, especially for the data generated by the experiment.

2.2.2 Main Proposer

For the same purpose, the Main Proposer is the scientist actually submitting the initial proposal and may differ from the Principal Investigator. If this is the case, the Main Proposer will have the responsibility of acting as the contact person for proposal authors (including communication of the outcome of the reviews) and the practical preparations for the experiment in case the proposal is awarded beamtime.

2.2.3 Proposers

The (Co-)Proposers are all scientists identified as authors in the proposal.

2.2.4 Participants in the experiment

The Participants are the scientists designated to take part in the actual measurements at the European XFEL facility. They may also differ from the authors of the proposal.

2.2.5 Sample coordinator

Designation of a sample coordinator must made at the proposal submission step. It is marked through a specific icon . This scientist will have the responsibility for all sample-related issues. Later, this selection can be changed on the A-form submission.

October 2021 18 of 43 XFEL.EU TN-2017-001-3.0

2.3 European XFEL proposal form

2.3.1 Choice of scientific instrument

Before filling in the proposal form, the choice of the scientific instrument (and, consequently, the relevant Proposal Review Panel) is made. Each Proposal Review Panel reviews all proposals submitted for allocation to one specific instrument. Only instruments available in a given call for proposals will be displayed in the relevant dropdown.

Once the step "save and continue" has been selected at the start of the form, it will not be possible to change the instrument(s) in this proposal any longer.

Figure 6: Choice of instrument (and complementary instrument for cross-instrument proposals)



2.3.2 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 proposal should be conducted on an additional EuXFEL instrument subsequently or in parallel, the selection of a complementary instrument is possible before filling in the proposal form.

Make sure that the proposal addresses the experiment sessions on both instruments exhaustively (including the part "Beam properties and instrument configuration". For scheduling reasons, the proposal will receive individual IDs on submission and will be reviewed by both instrument Proposal Review Panels concerned.

XFEL.EU TN-2017-001-3.0

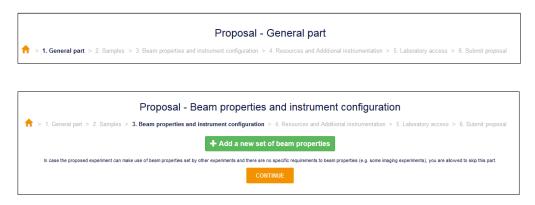
October 2021

CAUTION: The cross-instrument proposal option must **not** be used for aiming the submission of the same proposal to two different instruments—this will **not** increase the chances of allocation but may simply lead to withdrawal of one or both proposal(s) from the review process.

2.3.3 Navigation

Once you have opened the proposal form, the breadcrumb navigation at the top center enables you to navigate from one section of the form to the other, as shown in Figure 7. However, you have to create and save a "General part" before proceeding with other sections. It is recommended to fill in each section of the form sequentially, one section after the other.

Figure 7: Inactive (top) and active (bottom) breadcrumb navigation at the top of different parts of the proposal form



2.3.4 General part

2.3.4.1 General information

The "General part" of the proposal gives some basic information on the project and the scientists involved. Some general information, like affiliation to a User Consortium or the involvement of industrial users in the project is, requested for merely **statistical/informative** purposes and **has no influence on the ranking of the proposal**. The same applies to the selection of the scientific area, Horizon 2020 (H2020) challenges, or Helmholtz challenges, or statement on expected innovative impact of the project.

October 2021 **20** of **43** XFEL.EU TN-2017-001-3.0

In this part, you must define whether the proposal is a resubmission or the continuation of a previously submitted proposal. **Make sure you indicate the correct ID of the previous proposal of reference in the text box.**

2.3.4.2 Previous FEL experiments

Give information on previous experiments at FELs related to this proposal.

2.3.4.3 Previous FEL experience

Give details about proposers' experience at FELs, e.g. list of facilities at which they have worked already (as users or staff).

2.3.4.4 Instrument team contacted

If you have discussed with the instrument scientific team the feasibility of the conditions required by your experiment BEFORE submitting your proposal, please give details (e.g. name of team member, date).

2.3.4.5 Proposal continuation or resubmission

By selecting continuation or resubmission of a proposal, you will be requested to select the ID number of the relevant previous project(s) from a drop-down menu listing the ones submitted at an earlier stage. All existing ID numbers are visible to all UPEX users, but you will see only the titles of proposals to which you were already related in the past (e.g. as proposer or experiment team member) and for which you have viewing rights.

In case of a proposal continuation, it is mandatory to indicate the main objectives continued in the present proposals and, in case of a proposal resubmission, the main changes with respect to the preceding version.

2.3.4.6 Abstract

The abstract consists of a maximum of 1000 characters. This is the first information that the reviewers will see about your project.

2.3.4.7 Description of Proposed Experiment

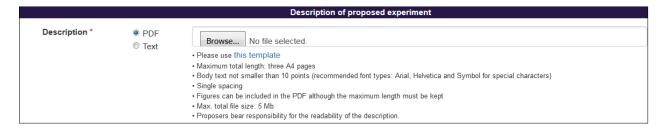
This part of the proposal is mandatory. Using the radio buttons in the form, you can choose between uploading the description to UPEX as a PDF (Portable Document Format, recommended in case of figures and/or formulas) or including the description as **text**, as shown in Figure 8. The RTF (Rich Text Format) form file for the preparation of the final PDF file is also accessible on your UPEX dashboard.

In order to to offer a better service to users, all European synchrotrons and free- electron lasers (FELs) have agreed upon a common list of proposal form labels at the end of 2018. The experiment description template in use at European XFEL was amended in May 2019 to reflect this standardization.

For more information about this, see:

http://www.wayforlight.eu/en/users/spf

Figure 8: Choosing between PDF upload and text descriptions in the "Description of proposed experiment" section of UPEX



2.3.4.7.1 Description of experiment – PDF upload option

An RTF file template is provided and it can be downloaded directly by clicking the link **Please Use This Template**.

Rules for using the PDF upload option:

- Maximum total length: Three A4 pages.
- Minimum body text size:10 points.

October 2021 **22** of **43**

XFEL.EU TN-2017-001-3.0

■ Recommended font types:

Arial, Helvetica, and Symbol (for special characters).

■ Line spacing:

Single spacing.

Figures:

May be included in the PDF as long as they do not exceed the page margins or maximum file size.

■ File size:

Maximum total file size of 5 MB.

Responsibility:

Proposers bear responsibility for the readability of the description.

Publications illustrating the scientific case should be added in this section. Mandatory information: title, authors (and their affiliations), journal name, volume, issue, and year of publication.

2.3.4.7.2 Description of experiment – Text option

A text form is provided for this option. You can then type (or paste) the answers to the relevant questions directly into the form. However, it is not possible to include figures or use symbols or special characters (other than Latin and Western Europe characters) in this section.

The maximum number of characters for this section, including headlines and questions, is 17 000. That is, your own text cannot exceed 16 650 characters when replacing the text already included in the form in square brackets ([...]) by the experiment description.

Publications illustrating the scientific case should be added in this section. Mandatory information: title, authors (and their affiliations), journal name, volume, issue, and year of publication.

2.3.4.7.3 Publications by the Proposers

This section has the purpose of giving information about the scientific activity of the Proposers related to the project detailed in the proposal.

XFEL.EU TN-2017-001-3.0

October 2021

List up to 15 articles, reports, and/or proceedings published by the Proposers over the past three years that are related to this proposal. If possible, include the DOI or PubMed ID.

NOTE: The "Publications by the proposers" and the "Publications illustrating the scientific case" sections are still under development and will evolve over the next few calls for proposals to become more user-friendly. Many thanks in advance for your patience.

2.3.4.7.4 Suggested reviewers to avoid

All proposals will be peer-reviewed, as detailed in the Terms of Reference of the European XFEL Proposal Review Panels (PRPs), and will be evaluated by Members of the PRPs and, if required, by external experts. In the textbox "Suggested reviewers to avoid", you may want to give information about scientists who could have a potential conflict of interest and should therefore not review the proposal.

2.3.4.7.5 Peaceful use of European XFEL facility

The European XFEL pursues research for peaceful purposes only. Please confirm by selecting the appropriate box that the present proposal exclusively aims at and promotes peaceful purposes. You cannot proceed with your proposal submission until you have electronically confirmed this.

2.3.5 Sample/Substance Sheets

Fill in one form for each sample and substance to be used in your experiment. List all samples and substances that you are planning to use in the experiment.

If your proposal is successful, after scheduling, you will be requested to confirm the samples or substances you intend to use in your experiment. Unilateral changes in the samples or substances mentioned in the experiment proposal are not acceptable. If, for serious reasons, the planned samples or substances are not available for the experiment and others need to be used, the EuXFEL Management Board will decide on the case after approval by the Safety and Radiation Protection group and a technical assessment by the instrument group supporting the experiment. In order to inform the EuXFEL

October 2021

XFEL.EU TN-2017-001-3.0

24 of 43

facility of this situation and request an authorization to replace a sample or substance, contact the EuXFEL User Office in writing and provide details. Ideally, this should happen at the stage of registration of the user group, in normal circumstances, four weeks before the experiment, and, in any case, not later than two weeks before the experiment. The proposers will be informed about the outcome of the change request as soon as possible.

Make sure you complete and save a sample sheet before you open a new one. After saving a complete sample sheet, you have the option of opening a new sample form, or cloning or deleting the sample sheet you are currently working on.

The Save button at the bottom enables you to save the form only if the data entered are complete. The Save and Continue button enables you to save the form if it is complete and move to the next step.

As a Main Proposer, you will be requested to certify that all details given in the Sample or Substance Sheet are complete and correct.

You will be requested to state whether a **specific sample requires long preparation** between notification of the outcome of the beamtime allocation process and the experiment (three months or longer). In this case, we will attempt to schedule your experiment with a delay of at least three months from the moment of notification. Note that this will create an additional scheduling constraint for your experiment. Consider that long delivery time for chemicals used in sample preparation may have a similar impact!

Each Sample and Substance Sheet must include a general part and <u>at</u>

<u>least one</u> of the following specific sections: biological/isolated from

biological substance, hazardous, nanomaterial, other samples or substances.

NO experiments with live animals and humans are permitted at EuXFEL.

The use of radioactive samples or substances is not feasible in early user operation. If you intend to prepare for using radioactive substances, pieces of equipment involving radiation, or sources later in steady operation, contact

the Safety and Radiation Protection group by email (expsaf@xfel.eu) well in advance in order to check about feasibility conditions in future runs.

2.3.6 Beam properties and instrument configuration

This part of the proposal form does not give any information on the actual properties available for each instrument in a specific allocation period. The actual information is available on the homepage of each scientific instrument and may change for each specific allocation period or run. In order to verify the feasibility conditions of your project, contact the scientific instrument groups.

2.3.7 Standard instrument configurations

An efficiency advantage can be established on some instruments with the development of "standard configurations". The goal is allowing user experiments to be grouped together back-to-back without involving a major change in setup every time. In addition, these will help provide a pathway to widen 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. Please refer to the call announcement and information on the instrument homepages and contact the instrument scientists for details about the available standard configurations.

2.3.8 Choice between standard and custom instrument configurations / beam properties

At the start of the instrument configuration and beam property section, you will have to choose between a standard configuration for the selected instrument, as advertised in the call (see above), or a custom (beam properties and instrument) configuration.

Figure 9: Choice of a standard configuration specific to the selected instrument

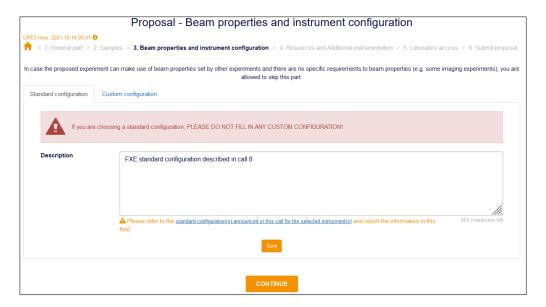
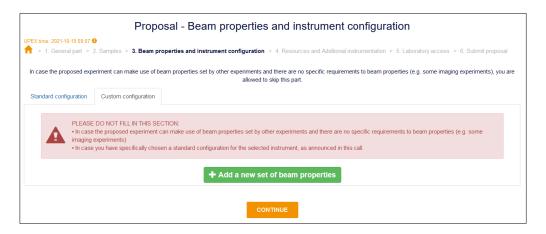


Figure 10: Choice of custom beam properties and instrument configuration



CAUTION: DO NOT FILL IN THIS SECTION:

- In case the proposed experiment can make use of beam properties set by other experiments and there are no specific requirements to beam properties (e.g. some imaging experiments).
- In case you have specifically chosen a standard configuration for the selected instrument announced in this call.

If you need specific beam properties and custom configuration information, it is possible to apply for a main set of beam properties and two secondary ones.



CAUTION: Multiple sets of beam properties may limit feasibility and allocation possibilities of your proposal.

2.3.8.1 Single pulse properties

Indicate the photon energy range that would make your experiment possible.

Refer to the specific range of each instrument in the allocation period of reference:

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

In addition, you must indicate the following:

- Bandwidth
- Pulse duration
- Pulse energy
- Spot size (diameter)

Prioritize each of the properties requested through the dropdown menu by selecting No Priority, Low Priority, High Priority.

Describe any special/additional requirements in the appropriate text box at the bottom of the section.

2.3.8.2 Requested pulse pattern

Refer to the information on each specific instrument for the relevant call:

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

In this section, you are requested to specify the number of pulses per train, the pulse train length, and the requirements on special patterns.

Add any special or additional requirements in the Special Pattern text box at the bottom of the section.

To edit any field contained in the Beam Properties and Instrument Configuration section, or to add new information, click the **green edit icon**. To delete the set of beam properties, click **red delete icon**.

Figure 11: Overview of a completed Beam Properties and Instrument Configuration section



2.3.9 Resources and Additional Instrumentation

In the Resources and Additional Instrumentation section, you are requested to give details about further resources and instrumentation needed for your experiment. Provide information that is as accurate as possible since, in addition to the review outcome, the planning of the proposal is based on this information.

In particular, provide information about **optical lasers**, **required detector configuration**, **sample delivery**, **and any other equipment you may need**. Enter **requirements about typical laboratory equipment** in the **Laboratory Access section**.

Generally, the use of your own instrumentation or equipment in the experiments requires feasibility, safety, and integration pre-assessment. If you are planning to include in your proposal user-supplied instrumentation or equipment, please contact the relevant scientific instrument team well before proposal submission in order to verify feasibility and declare this in the specific field for each piece of equipment. Below you will find rules for user-supplied instrumentation and equipment.

2.3.9.1 Rules for user-supplied instrumentation and equipment

In general, user-supplied equipment, instrumentation, and tooling shall only be used in experiments after testing and agreement by EuXFEL. Complete information about user-supplied equipment, instrumentation and tooling shall be provided at the proposal stage at the latest (cf. (a) below).

- (a) If the Principal Investigators, Proposers, and/or Participants in an experiment plan to bring their own equipment to use at EuXFEL, either on the instrument or in the user laboratories for sample preparation, this must be discussed with the relevant scientists of the instrument or laboratory well before proposal submission. If needed, the scientists will then address the relevant experts from the EuXFEL support teams. The equipment shall be described in the proposal and will be subject to acceptance by EuXFEL in the framework of the feasibility checks about the projects.
- (b) Equipment needs to be checked by the Safety and Radiation Protection group, and Principal Investigators, Proposers, and /or Participants may be requested to provide a risk analysis of the equipment, depending of the outcome of the proposal evaluation. All material, including samples and equipment brought to the EuXFEL facility remains entirely the responsibility of the Principal Investigators, Proposers, and Participants. Depending on the proposal evaluation, further tests or modifications to the equipment could be required to adapt it for use at the EuXFEL facility well before the experiment, generally at the costs of the user group.

2.3.9.2 Optical lasers

Click the green Add Optical Laser button in order to open the form to enter the required parameters: Description of Laser Usage, Wavelength, Pulse Duration, Pulse Energy, Focus/Beam Size, Delay Range, and Information or Required Pattern. Special requirements should be detailed in the text box.

For information about maximum laser performance, refer to Table 2, which summarizes set points at the start of operation of the EuXFEL facility.

For further information, please contact the instrument scientists before proposal submission.

Table 2: Basic European XFEL pump–probe laser parameters and set points (courtesy of M. Lederer, Optical Lasers group)

λ	800 nm	1030 nm
τΦΩΗΜ	15–300 fs (nearly transform- limited)	< 1 ps or 400 ps (chirped)

Set point	f _{rep} [MHz]	E _{pulse} [mJ] @ 800 nm	E _{pulse} [mJ] @ 1030 nm
1	4.5	0.05	1
2	1	0.2	4
3	0.2	1	20
4	0.1	2	40

Notes:

- The laser pulses are synchronized to the X-ray pulses.
- Repetition rate and energy set points 1–4, in combination with wavelength and pulse-width settings, correspond to fixed laser set points. Arranging for a different set point requires a configuration change of the laser.
- From any set point repetition rate, pulse patterns can be selected as required, including single pulse selection on both wavelengths.
- Set points with dual wavelength output can be arranged on request.
- Variable attenuation is available on request.
- Beams are close to diffraction-limited.
- Harmonics are possible on request.
- For further details, contact EuXFEL before submitting your proposal.

2.3.9.3 Required detector configuration

Provide information and a justification on the planned use of detector(s) during your experiment:

- Detector type/name
- Sample-detector distance
- Planned use and special requirements (textbox)

For specific instructions, see the on relevant instrument page:

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

2.3.9.4 Sample delivery

Describe the required sample delivery in the text box.

2.3.9.5 Other equipment

This part must be completed **after consultation of the instrument scientists.** Provide details about the agreed requirements in the form.

2.3.10 Laboratory access

To fill out the Laboratory Access section correctly, refer to the **information about the EuXFEL user laboratories** available on our website:

https://www.xfel.eu/users/experiment_support/user_labs

2.3.10.1 Laboratory workspace

In this section, you state the type of laboratory working space to which you are requesting (Biology Laboratory Risk Group 1 or 2 or other laboratories) with more detailed information that is useful for scheduling purposes (e.g. estimate of time needed at which type of working space, description of work, frequency of work during beamtime).

The size of a working space amounts to 1.2 or 1.5 metres each and, for biology laboratories, a max. of 4 working spaces can be requested at the same time.

October 2021 32 of 43 XFEL.EU TN-2017-001-3.0

2.3.10.2 Laboratory equipment

Independently of the access to workspace in a specific lab, you can separately request access to specific laboratory equipment.

To be able to fill out this section correctly, refer to the information about the EuXFEL user laboratories available on our website:

https://www.xfel.eu/users/experiment_support/user_labs

Note that exclusive use of the equipment is not guaranteed.

In this section, you can also specify if you need to **access to gases** (Ar, N_2 , O_2 , CO_2 , pressurized air, or other).

2.4 Special proposals

2.4.1 Protein Crystal Screening (PCS) proposals

Liquid jet injection is the most used sample delivery method for serial-femtosecond crystallography of proteins at the SPB/SFX instrument at EuXFEL. The complexity of sample preparation and injection still leads to the loss of valuable beamtime during user experiments. A protein crystal screening (PCS) process is being introduced, which combines sample characterization and injection tests in the laboratories, followed by screening beamtimes at the SPB/SFX instrument. Specific proposals, submitted in the user portal UPEX, will be selected after peer review and feasibility and safety checks.

A specific ad hoc proposal form is available in dedicated PCS calls, typically taking place at the same time as regular calls.

The proposal form includes a general part, whereas the experiment description focuses on the proposed sample(s) and their scientific relevance:

- Maximum total text length: 1/2 A4 pages
- Body text not smaller than 10 points (recommended font types: Arial, Helvetica, and Symbol for special characters)
- Single spacing
- Figures can be included in the PDF although the maximum text length must be kept
- Max. total file size: 5 Mb
- Proposers bear responsibility for the readability of the description.

The PCS proposal form also includes a section on sample and substances in which, in addition to the usual information requested in the regular sample sheet, details on the protein crystals are requested.

3 Registering for experiments in UPEX

3.1 Registration of Experiment Team (A-form) and Personal Arrival Form (PAF)

3.1.1 A-form (Arrival Form)

The A-form is the electronic form used for registering the experiment team and confirming samples and substances to be used in the experiment.

Only the Main Proposer fills in the A-form. He/she can add to the A-form only already registered users; therefore, all members of the experiment team must be registered on the User Portal to the European XFEL (UPEX). It is the responsibility of the Main Proposer to make sure that all prospective members of the team create their personal accounts in UPEX in a timely fashion and accept the latest versions of UPEX user policies, terms, and conditions. The Main Proposer should also inform the team members that it is mandatory to successfully complete the needed user safety training before coming to our facility.

Currently, due to the COVID-19 pandemic, deviations from the usual rules for registration and access are required. The guidelines for participation in user operation during the COVID-19 pandemic have to be followed. "Remote" user access for all experiments is considered as the general rule. Any exception requires prior authorization, based on the evaluation of the necessity to allow onsite users for a specific experiment. These requests are provided by the Main Proposers and/or Principal Investigator to the User Office. If the authorization is requested for more than two users, a detailed written justification is mandatory.

XFEL.EU TN-2017-001-3.0

October 2021

The link to the active A-form is available to the Main Proposer in UPEX, (Role: Normal User), on the dashboard (left menu), next to the name and ID of the scheduled proposal.

In addition to the registration of the experiment team, the A-form includes the following:

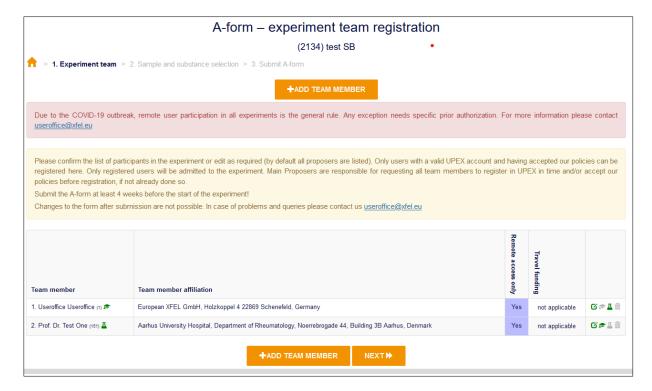
- Confirmation of samples/substances to be used during experiments (to be chosen among the samples/substances included in the original proposal).
 Please refer to our sample policy for detailed information.
- Designation of onsite users. To appoint onsite users, please contact the User Office by email with the names of the onsite users. If the authorization is requested for more than two users, a detailed written justification is mandatory. After authorization is given, we will set the onsite users in the submitted A-form and contact them by email regarding further arrangements.
- Designation of funded users. Detailed information about eligibility criteria and travel funding under <u>user travel regulations</u>. To appoint funded users, please contact the User Office by email (can be done together with appointment of the onsite users—please see previous point).
- Designation of remote-access users.
 - Designation of group coordinator on site (if there are changes with respect to the selection made on proposal submission)— marked by a specific icon —can be managed from the A-from
- Designation of sample coordinator (if there are changes with respect to the selection made on proposal submission)—marked by a specific icon
 —can be managed at the A-form step.

The User Office will set the onsite participants and funded users in the A-from after authorization is given.

The A-form must be completed and submitted at least four weeks before the start date of the experiment. Timely submission is in the interest of the user team. This is particularly crucial for practical arrangements (access,

accommodation, and travel support), computing accounts, and other aspects of the experiment support. If submissions are late, the User Office cannot guarantee that the requested support is provided.

Figure 12: Managing group coordinator and sample coordinator from the A-form



3.1.2 Personal Arrival Form (PAF)

The Personal Arrival Form is the electronic form that each experiment participant has to fill in before arriving at our facility.

After the Main Proposer submits the A-form, all authorised onsite participants will be able to fill in and submit the Personal Arrival form. The link to this form can be found on the normal user UPEX dashboard. In this form, each participant has to provide information about the duration of their stay and may request support for practical arrangements (travel and accommodation for funded users, invitation letters for visa purposes, site access permissions, etc.).

The Personal Arrival Forms must be submitted at least 10 days before the start of the experiment. Otherwise, the User Office cannot guarantee that the requested support will be provided.

3.1.3 Lab access requests

Each onsite user can request lab access via a specific checkbox in the Personal Arrival Form (PAF). After submission, the relevant account will be exported to Booked, the user lab management system.

3.2 Attribution of responsibilities within the user team

Please note that the attribution of functions in the proposal submission and allocation process within the user team has to be done through the selection of the relevant scientist at the proposal stage. Each scientist mentioned in a proposal with the role of Principal Investigator, Main Proposer, or Co-Proposer receives an email confirmation from UPEX on proposal submission.

3.2.1 Principal Investigator

Besides being in most cases the lead researcher or one of the lead researchers of the project addressed in the proposal, for the purpose of access to the EuXFEL facility, the Principal Investigator is specifically identified among the authors of the proposal and bears exclusive long-term responsibility for experiment, especially for the data generated by the experiment.

For more information, refer to our Scientific Data Policy:

https://in.xfel.eu/upex/docs/upex-scientific-data-policy.pdf

3.2.2 Main Proposer

For the same purpose, the Main Proposer is the scientist actually submitting the initial proposal and may differ from the Principal Investigator. If this is the

October 2021

XFEL.EU TN-2017-001-3.0

38 of 43

case, the Main Proposer will have the responsibility of acting as the contact person for proposal authors (including communication of the outcome of the reviews) and the practical preparations for the experiment in case the proposal is awarded beamtime, including registration of participants in the experiment and confirmation of samples and substances used in the experiment.

3.2.3 Co-Proposers

The Co-Proposers are all scientists identified as authors in the proposal.

3.2.4 Participants in the experiment

The Participants are the scientists designated to take part in the actual measurements at the EuXFEL facility. They may differ from the authors of the proposal although this is not recommended.

4 Feedback

4.1 Experiment reports

4.1.1 General rules for experiment reports

As soon as the last shift of a beamtime has been completed, a link to the experiment report template will appear on the user dashboard of the Main Proposer in UPEX, in the "Feedback" section:

https://in.xfel.eu/upex

Submission of the experiment report is required between 3 to 6 months after end of last shift of the experiment.

However, in the event of new proposals or continuation proposals by same scientists (as Main Proposers and/or Principal Investigators):

- You must submit experiment reports via the User Portal to the European XFEL (UPEX) about all previous measurement(s) by the deadline for experiment reports indicated in the relevant call for proposals, including
 - Those carried out close to the proposal submission deadline
 - Experiments whose scientific area or instrument is different from those relevant to your new proposal
- You must supply a reference to this report in your new proposal(s) by indicating the corresponding experiment ID in the "continuation/resubmission" field in the General Part of the new proposal.

If one experiment has been allocated beamtime on several occasions, you can submit a single full report that covers the totality of the beamtime allocated for this experiment. However, intermediate reports are required in case of submission of new proposals or continuations of previous beamtimes by the same scientists (as Main Proposers and/or Principal Investigators).

October 2021

XFEL.EU TN-2017-001-3.0

Experiment reports are to be directly uploaded to UPEX. Later updates must be emailed to useroffice@xfel.eu.

4.1.2 Instructions for uploading your experiment report to UPEX

Format instructions for the report:

- Maximum total length: Two A4 pages
- Body text not smaller than 10 points (recommended font types: Arial and Helvetica, as well as Symbol for special characters)
- Single spacing
- Figures can be included in the PDF, although the maximum length must be kept
- Max. total file size: 5 Mb
- Proposers bear responsibility for the readability of the description.

4.2 Feedback form

All users are welcome to share observations, recommendations, ideas, and general comments related to their experience at the EuXFEL. We sincerely appreciate all advice aiming at the improvement of the quality of our service.

For this purpose, a specific form is available in the "Feedback" section of the standard user dashboard in UPEX.

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Special thanks go to the user office colleagues in many facilities in Europe, in particular Daniela Unger and her team at DESY Photon Science for their constant competent help and advice as well as Stefan Janssen and his team at PSI for their valuable support and for providing the Digital User Office software from which UPEX was developed.

B Useful email contacts

EuXFEL User Office:	useroffice@xfel.eu
SASE1 scientific instruments:	FXE (Femtosecond X-ray experiments): <u>christopher.milne@xfel.eu</u>
	SPB/SFX (Single Particles, Clusters, and Biomolecules / Serial Femtosecond crystallography): spb.sfx@xfel.eu
SASE2 scientific instruments:	HED (High Energy Density Matter): ulf.zastrau@xfel.eu
	MID (Materials Imaging and Dynamics): mid- info@xfel.eu
SASE3 scientific instruments:	SCS (Spectroscopy and Coherent Scattering): scs@xfel.eu
	SQS (Small Quantum Systems): michael.meyer@xfel.eu
Sample Environment group and user labs:	sample.environment@xfel.eu