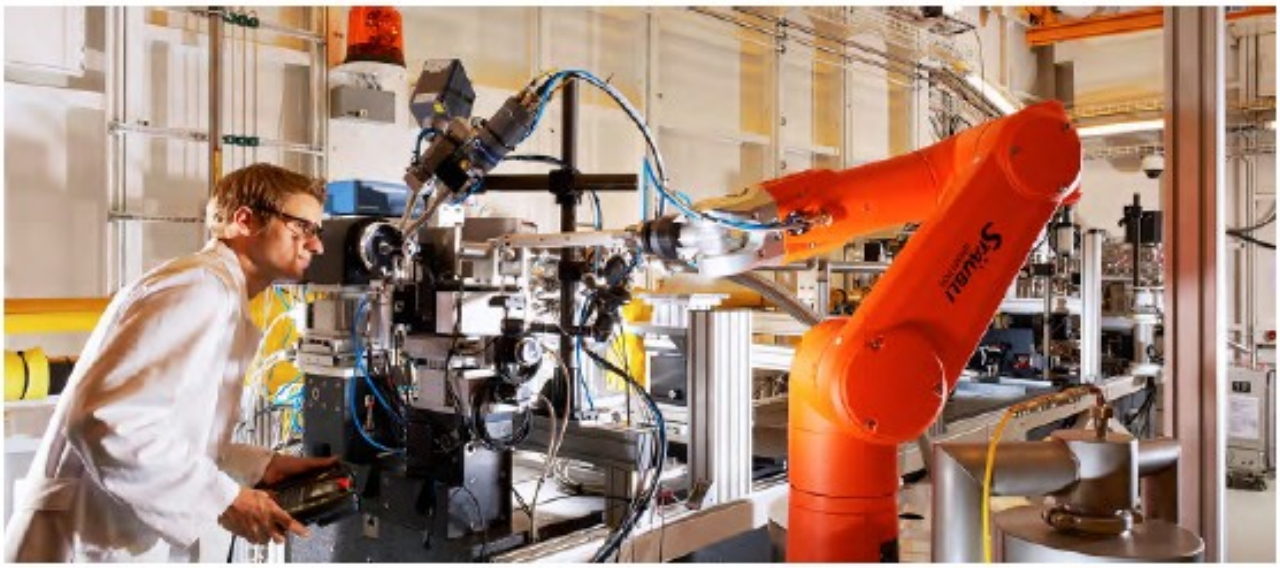
How to Perform Your Experiment at P11



This tutorial should help you to perform your experiment at beamline P11@PETRAIII.
More detailed information on the technical parameters of P11 and the research conducted at our beamline can be found at our webpage:
https://photon-science.desy.de/facilities/petra_iii/beamlines/p11_bio_imaging_and_diffraction/

If you have further questions please do not hesitate to contact your P11 staff:

Anja (phone: +49 40 8998 91775; email: anja.burkhardt@desy.de)
Eva (phone: +49 40 8998 96105; email: eva.crosas@desy.de)
Sofiane (phone: +49 40 8998 94620; email: sofiane.saouane@desy.de)
Johanna (phone: +49 40 8998 95756; email: johanna.hakanpaeae@desy.de)

Checklist

This list contains important items which need to be addressed before you can start your experiment at P11:

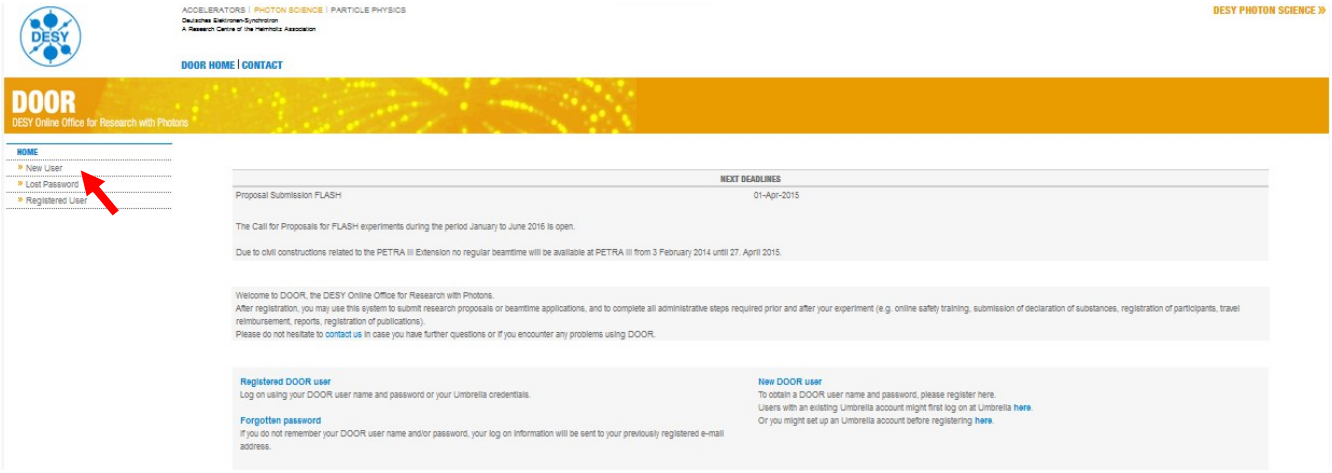
	Status
1) Declaration of substances submitted	
2) All participants of the experiment registered	
3) Safety training passed	
4) Certificate (printout) from the safety training sent to the Users' Office	
5) Local contact informed about arrival at P11	
6) DACHS card (badge) picked up	
7) Beam shutter permission obtained	

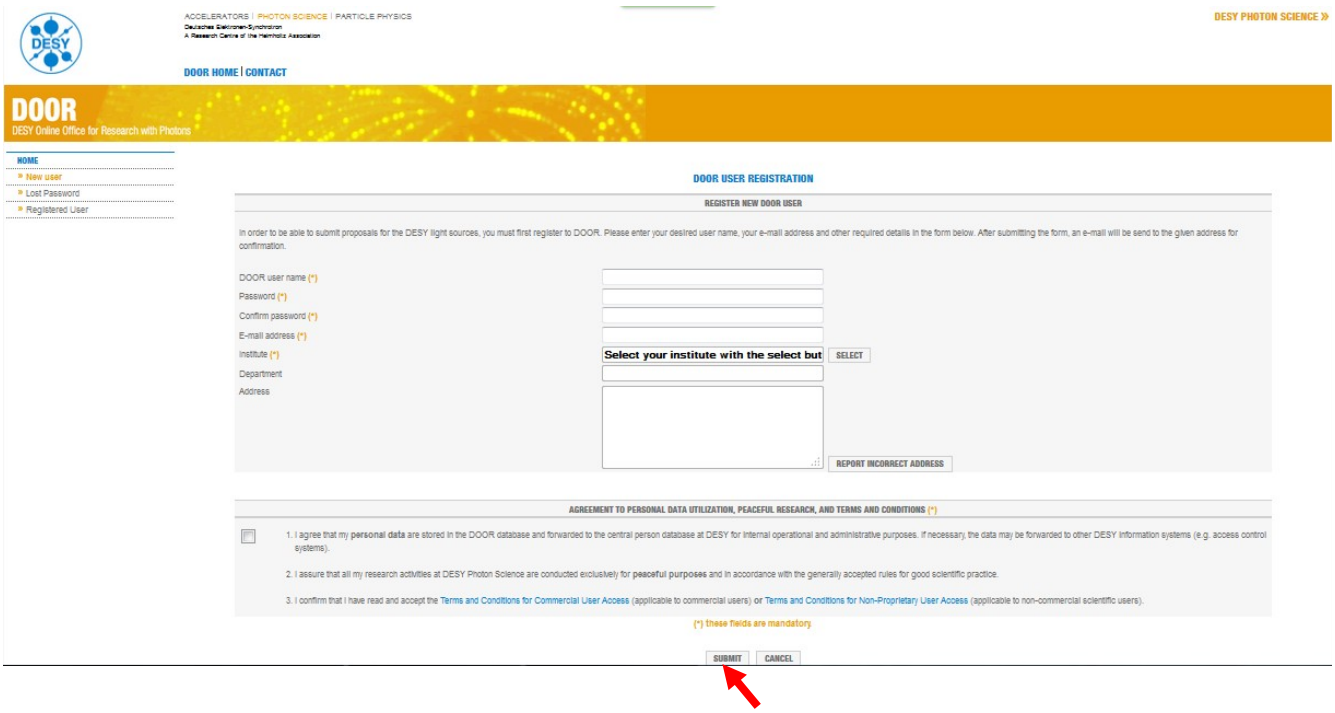
I. Before Your Arrival

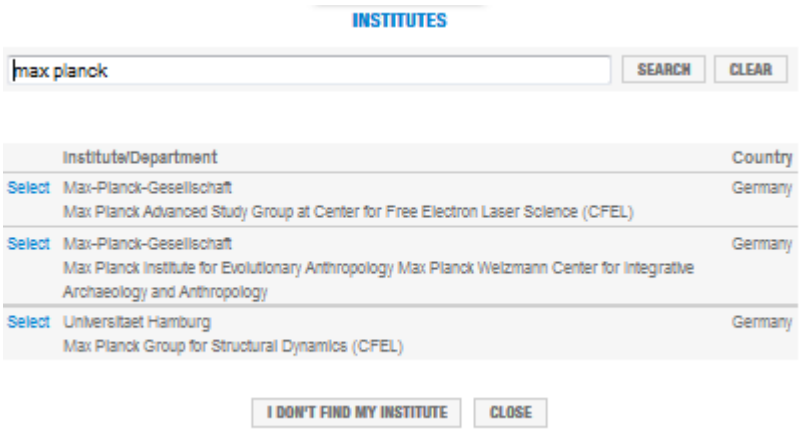
I.1. DOOR Registration

You are only allowed to apply for beamtime and perform your experiment at DESY with a valid DOOR account. Please register at DOOR (DESY Online Office for Research with Photons) via https://door.desy.de/door/index.php as follows:

a) Click on ‘New User’
b) Complete the registration form (Fields marked with (*) are mandatory).
c) Select your institute from the drop-down list. If you don’t find your institute in the database please contact the Photon Science Users' Office via photon-science@desy.de.
d) Submit the completed form




ACCELERATORS | PHOTON SCIENCE | PARTICLE PHYSICS
Deutsches Elektronen-Synchrotron
A Research Centre of the Helmholtz Association
DESY PHOTON SCIENCE »
DOOR HOME | CONTACT
DOOR
DESY Online Office for Research with Photons
HOME
» New user
» Lost Password
» Registered User
DOOR USER REGISTRATION
REGISTER NEW DOOR USER
In order to be able to submit proposals for the DESY light sources, you must first register to DOOR. Please enter your desired user name, your e-mail address and other required details in the form below. After submitting the form, an e-mail will be send to the given address for confirmation.
DOOR user name (*)
Password (*)
Confirm password (*)
E-mail address (*)
Institute (*)
Select your institute with the select but
SELECT
Department
Address
REPORT INCORRECT ADDRESS
AGREEMENT TO PERSONAL DATA UTILIZATION, PEACEFUL RESEARCH, AND TERMS AND CONDITIONS (*)
1. I agree that my personal data are stored in the DOOR database and forwarded to the central person database at DESY for internal operational and administrative purposes. If necessary, the data may be forwarded to other DESY information systems (e.g. access control systems).
2. I assure that all my research activities at DESY Photon Science are conducted exclusively for peaceful purposes and in accordance with the generally accepted rules for good scientific practice.
3. I confirm that I have read and accept the Terms and Conditions for Commercial User Access (applicable to commercial users) or Terms and Conditions for Non-Proprietary User Access (applicable to non-commercial scientific users).
(*) these fields are mandatory.
SUBMIT
CANCEL

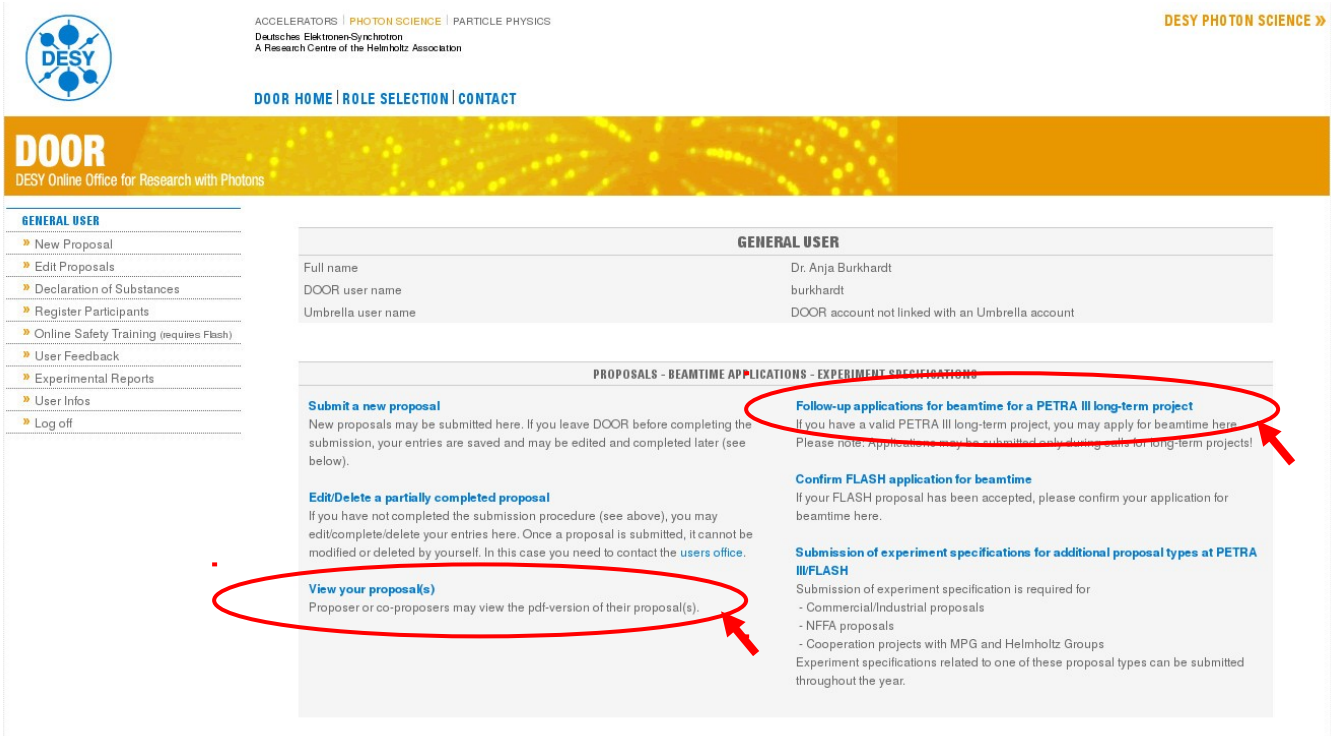

INSTITUTES
max planck
SEARCH
CLEAR
Institute/Department
Country
Select
Max-Planck-Gesellschaft
Max Planck Advanced Study Group at Center for Free Electron Laser Science (CFEL)
Germany
Select
Max-Planck-Gesellschaft
Max Planck Institute for Evolutionary Anthropology Max Planck Weizmann Center for Integrative Archaeology and Anthropology
Germany
Select
Universitaet Hamburg
Max Planck Group for Structural Dynamics (CFEL)
Germany
I DON'T FIND MY INSTITUTE
CLOSE

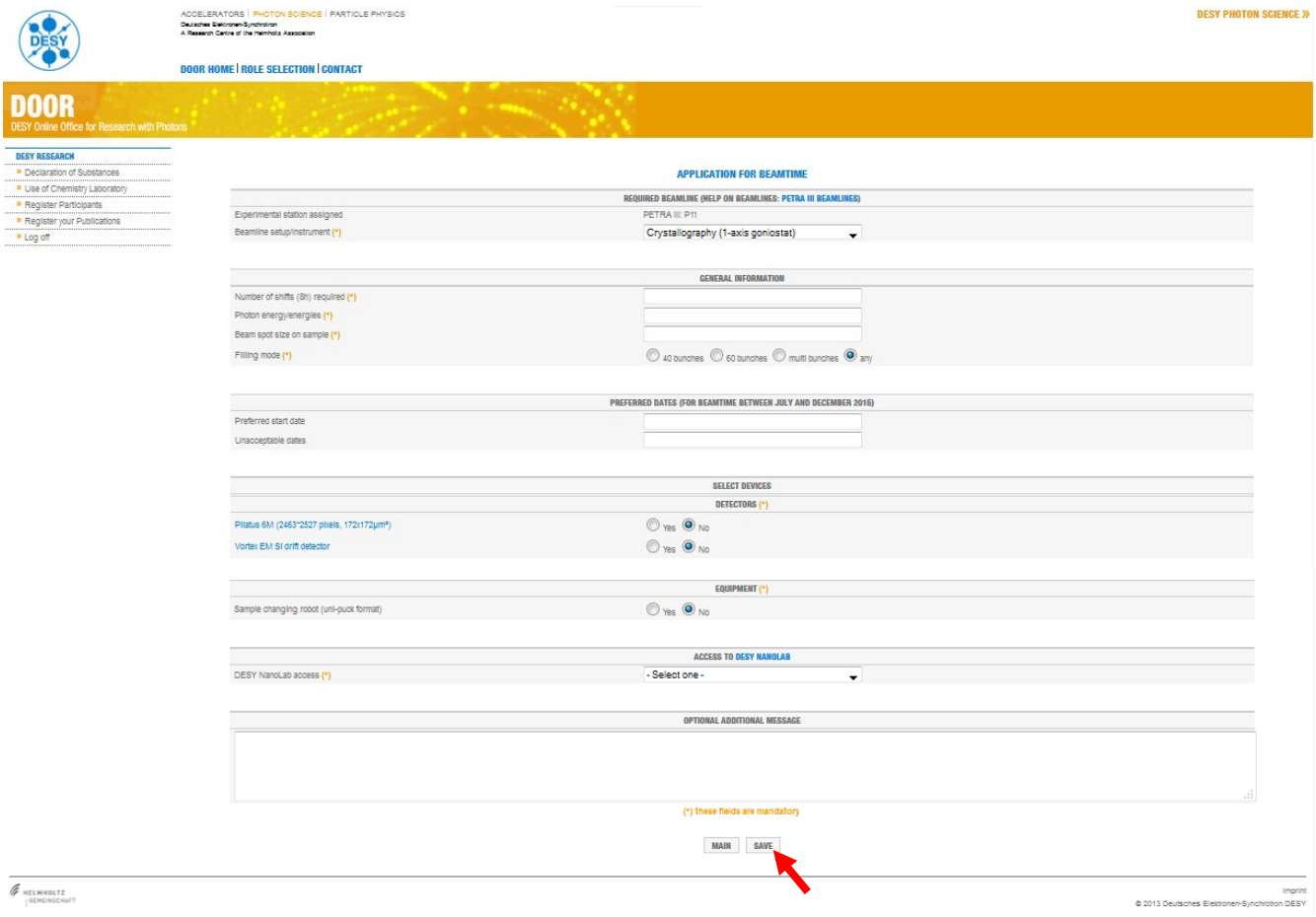
I.2. Beamtime Application

Beamtime applications need to be submitted via DOOR at least 4 weeks before you wish to perform your experiment at P11. This applies also for the 2nd, 3rd and 4th beamtime in the framework of a long-term proposal (the beamtime application for the 1st beamtime is submitted together with the proposal).
Beamtime applications for regular DOOR proposals are submitted together with the proposal. Please keep in mind, that according to the current DESY guidelines for PETRA III each regular DOOR proposal is valid for one beamtime at one beamline only (for more information please check here: http://photon-science.desy.de/users_area/users_guide/index_eng.html).

Shift schedule:	Morning shift:	09:00 – 17:00
	Afternoon shift:	17:00 – 01:00
	Night shift:	01:00 – 09:00

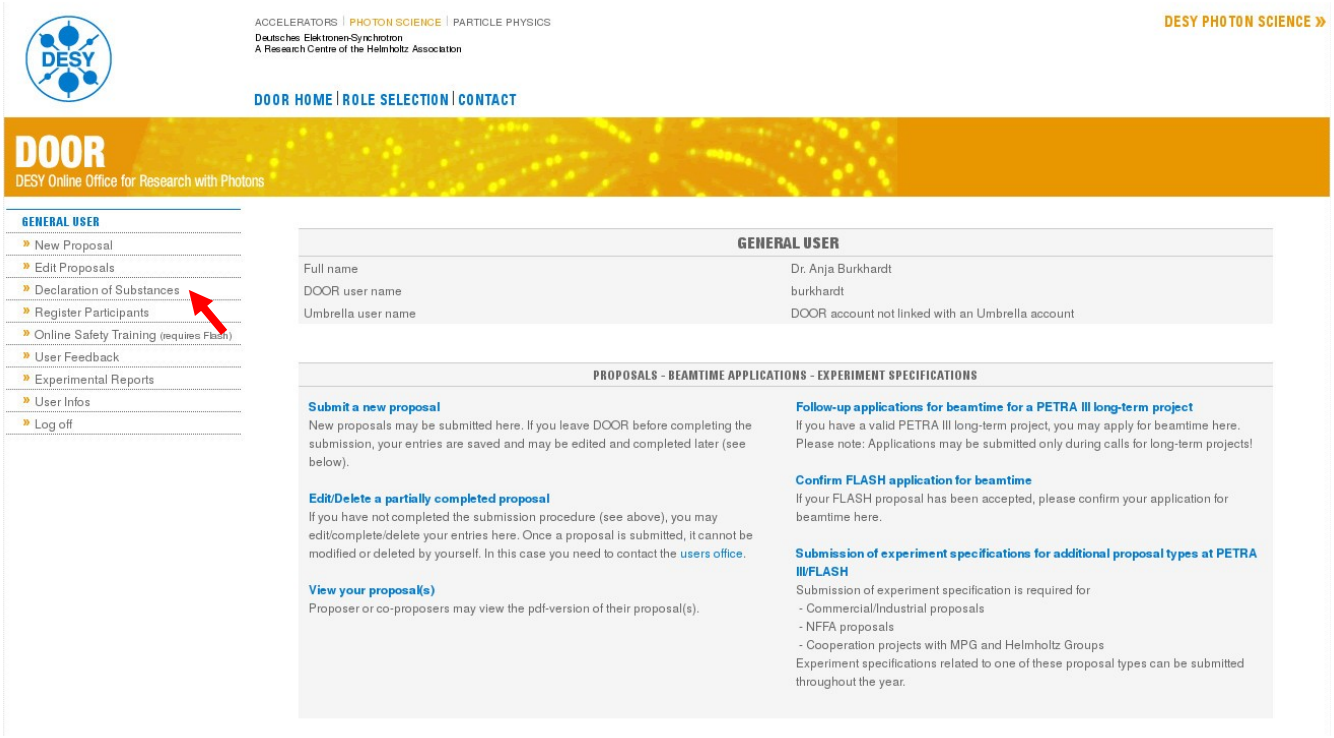
Due to the service shifts on Wednesday the night shift from Tuesday to Wednesday already ends at 7:00. This also applies to night shifts preceding shutdowns.

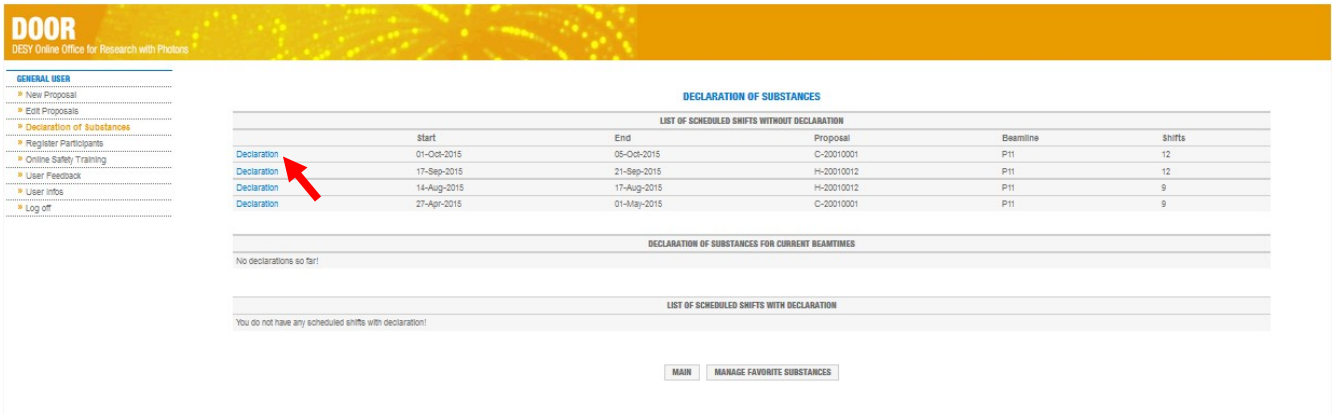




Complete the application form and submit it (All fields marked with (*) are mandatory.).

I.3. Declaration of Substances





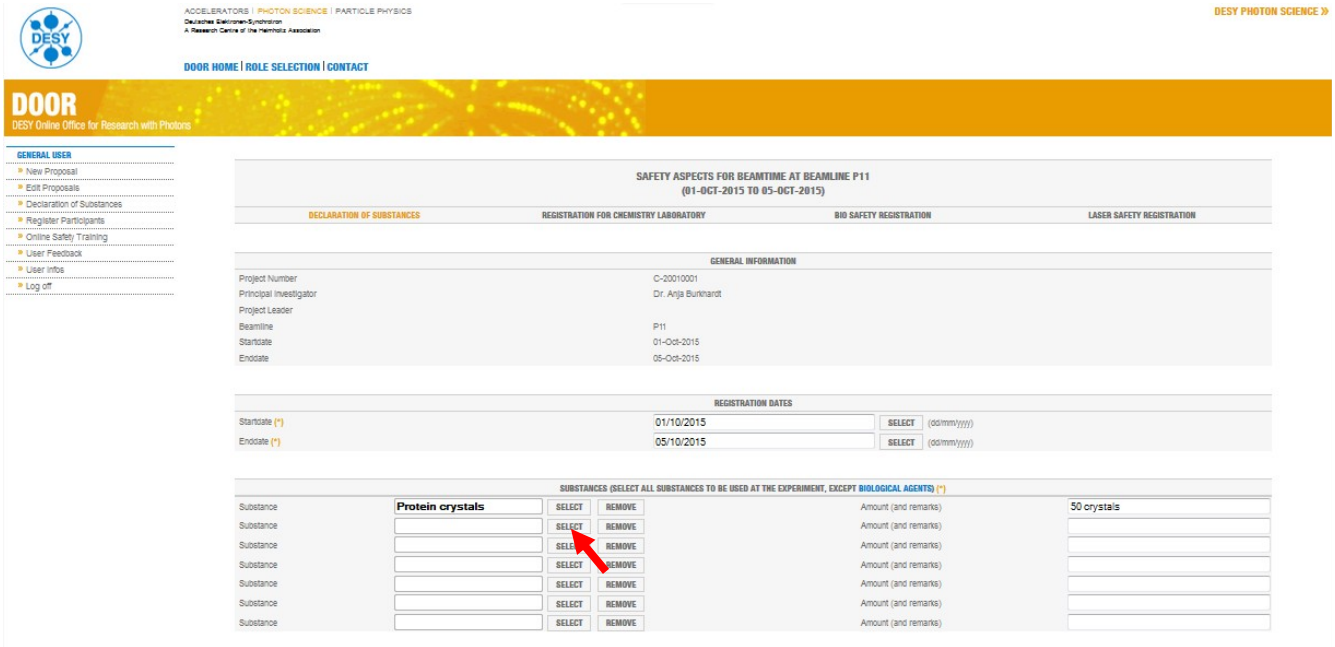
Fill in the mandatory fields (marked with (*)) and submit the completed form. To enter a list of protein crystals in the declaration form you may proceed as follows:
a) Click on ‘Add’ in the ‘Substance’ menu
b) Search for ‘protein crystals’ in the data base
c) Determine the safety category of your samples and select the corresponding ‘protein crystal’ entry.

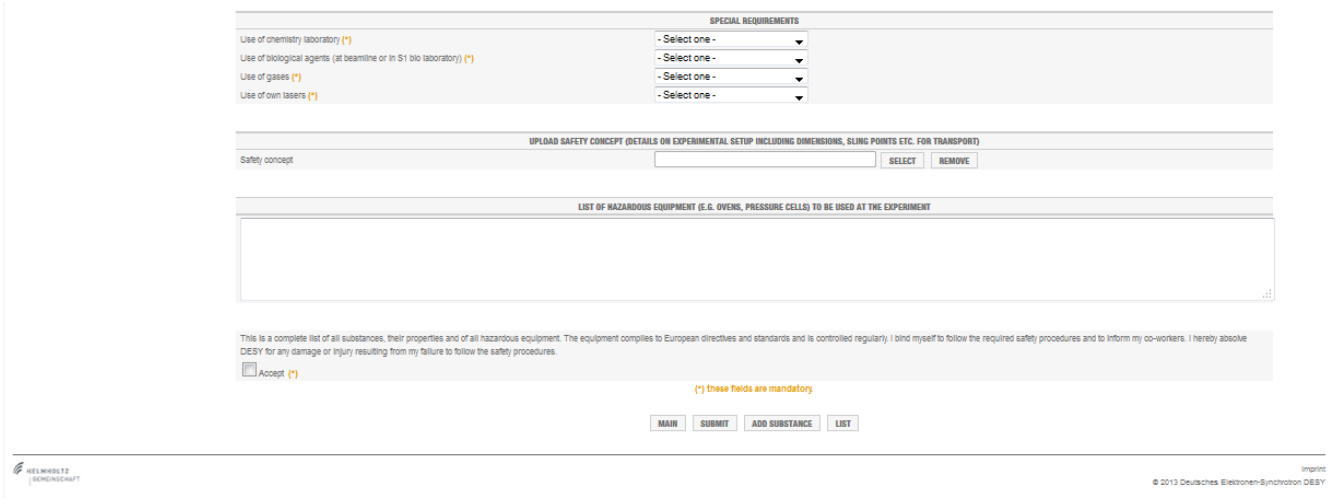
Entry	*Safety Category*
Protein crystals	Harmless, non-toxic, non-infectious
Protein crystals Inf.	Infectious. These are proteins which need to be classified as a biological agent according to the BioStoffV e.g. agents associated with transmissible spongiform encephalopathy, such as prions.
Protein crystals toxic	Toxic

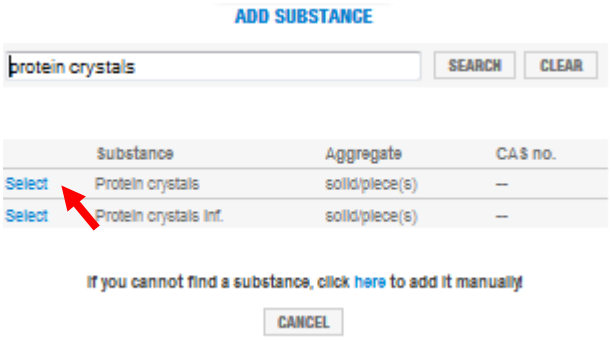
In case your sample does not fit to any of the available entries please create a new entry.

d) Specify the number of protein crystals you are going to measure in the ‘Amount and remarks’ field.
e) Upload a PDF document containing a list of all your samples in the ‘Safety concept’ menu. Please refer to this detailed list in the ‘Amount and remarks’ field via e.g. ‘details see safety concept’.

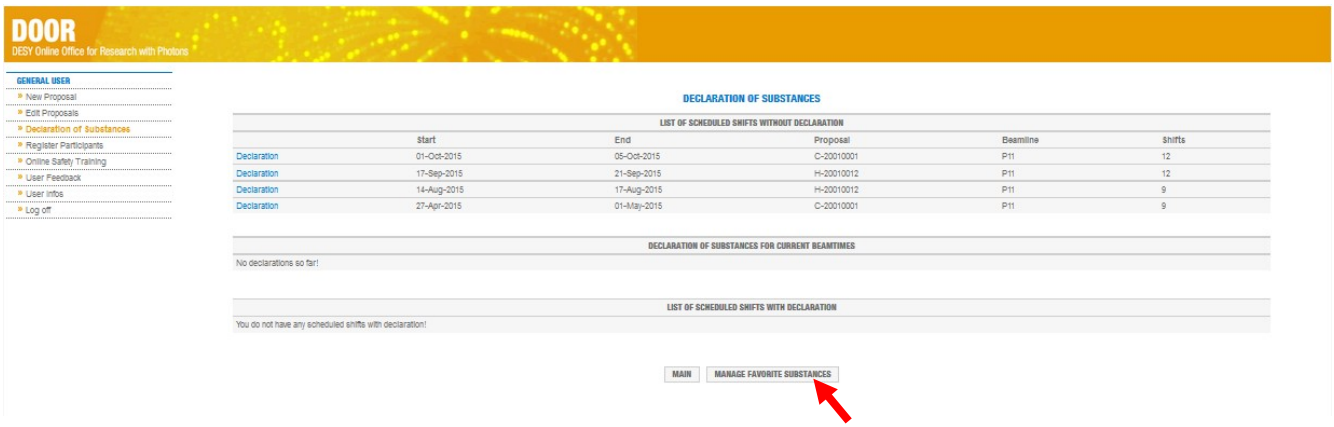
Please indicate also if any laboratory, gases or lasers are needed for your experiment. Please note that "chemistry laboratory" corresponds to the general chemistry lab at PETRA III (L031/032) and does NOT stand for the P11 user lab (L047). The latter can be accessed without further registration by every P11 user who has passed the corresponding safety training (see section 1.5).





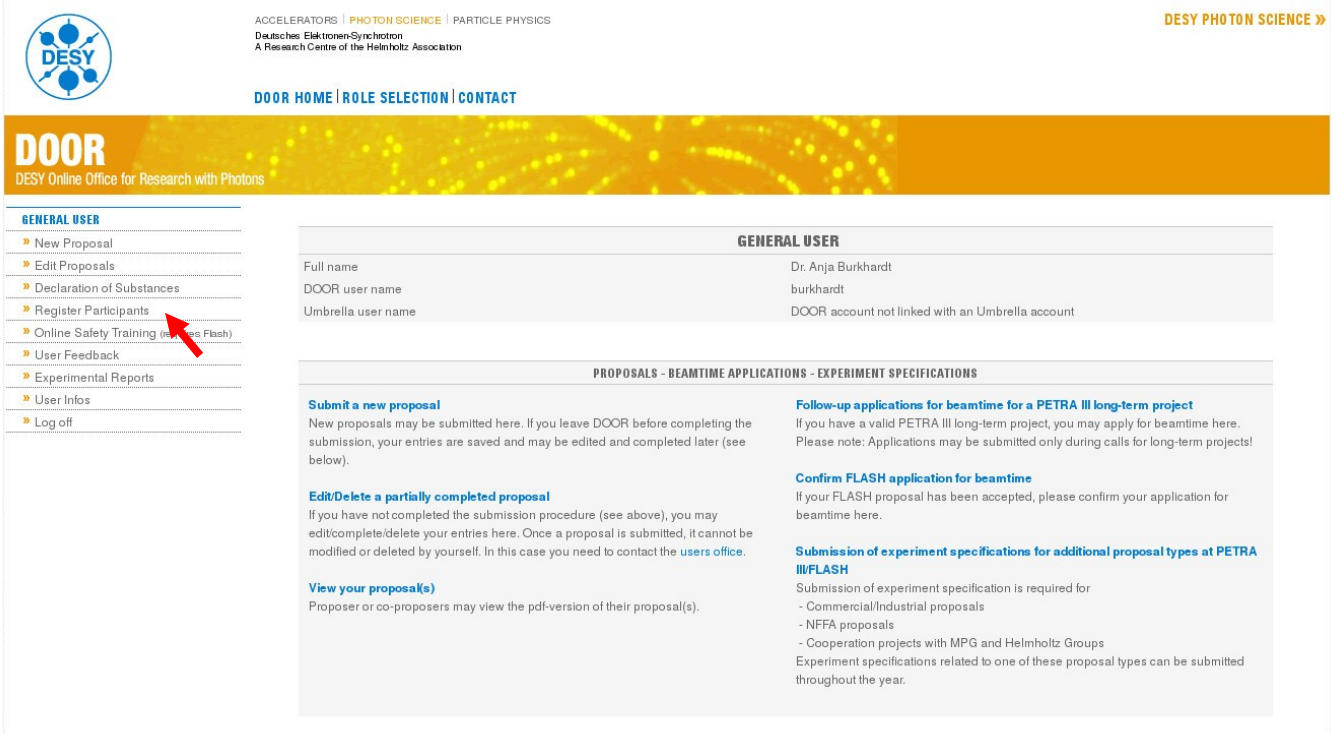


If you are frequently visiting P11 and are using the same chemicals or biological agents for every experiment you might want to create a list of favorite substances.

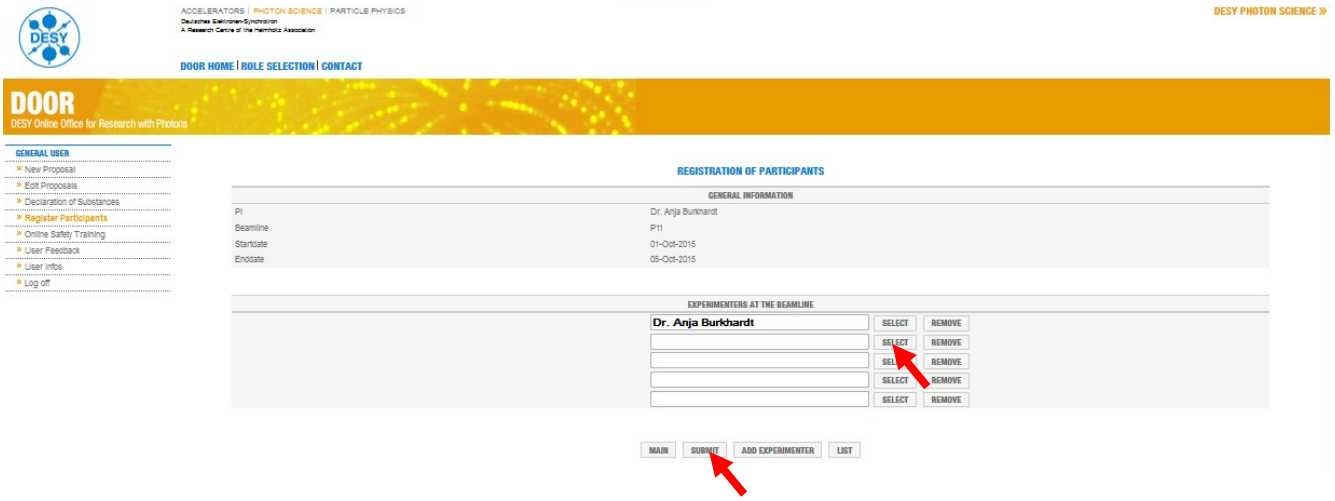


I.4. Register Participants

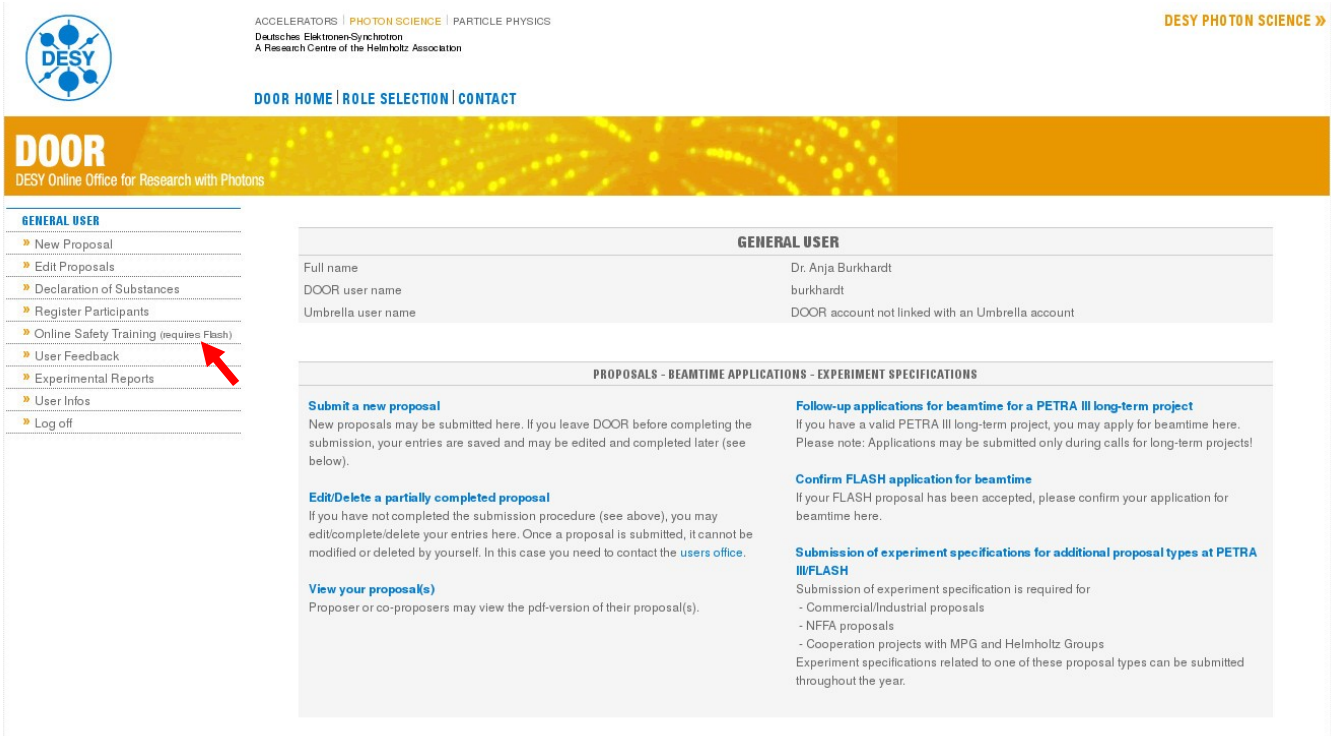
Register all persons participating in your experiment. This also includes the registration for the on-site safety training. Only people registered in DOOR can be added to the list of participants.




ACCELERATORS | PHOTON SCIENCE | PARTICLE PHYSICS
Deutsches Elektronen-Synchrotron
A Research Centre of the Helmholtz Association
DESY PHOTON SCIENCE »
DOOR HOME | ROLE SELECTION | CONTACT
DOOR
DESY Online Office for Research with Photons
GENERAL USER
» New Proposal
» Edit Proposals
» Declaration of Substances
» Register Participants
» Online Safety Training
» User Feedback
» User Infos
» Log off
REGISTRATION OF PARTICIPANTS
LIST OF SCHEDULED SHIFTS WITHOUT REGISTRATIONS
Start
End
Proposal
Beamline
Shifts
Register
01-Oct-2015
05-Oct-2015
C-20010001
P11
12
Register
17-Sep-2015
21-Sep-2015
H-20010012
P11
12
Register
14-Aug-2015
17-Aug-2015
H-20010012
P11
9
Register
27-Apr-2015
01-May-2015
C-20010001
P11
9
REGISTRATIONS OF PARTICIPANTS FOR CURRENT BEAMTIMES
No registrations so far!

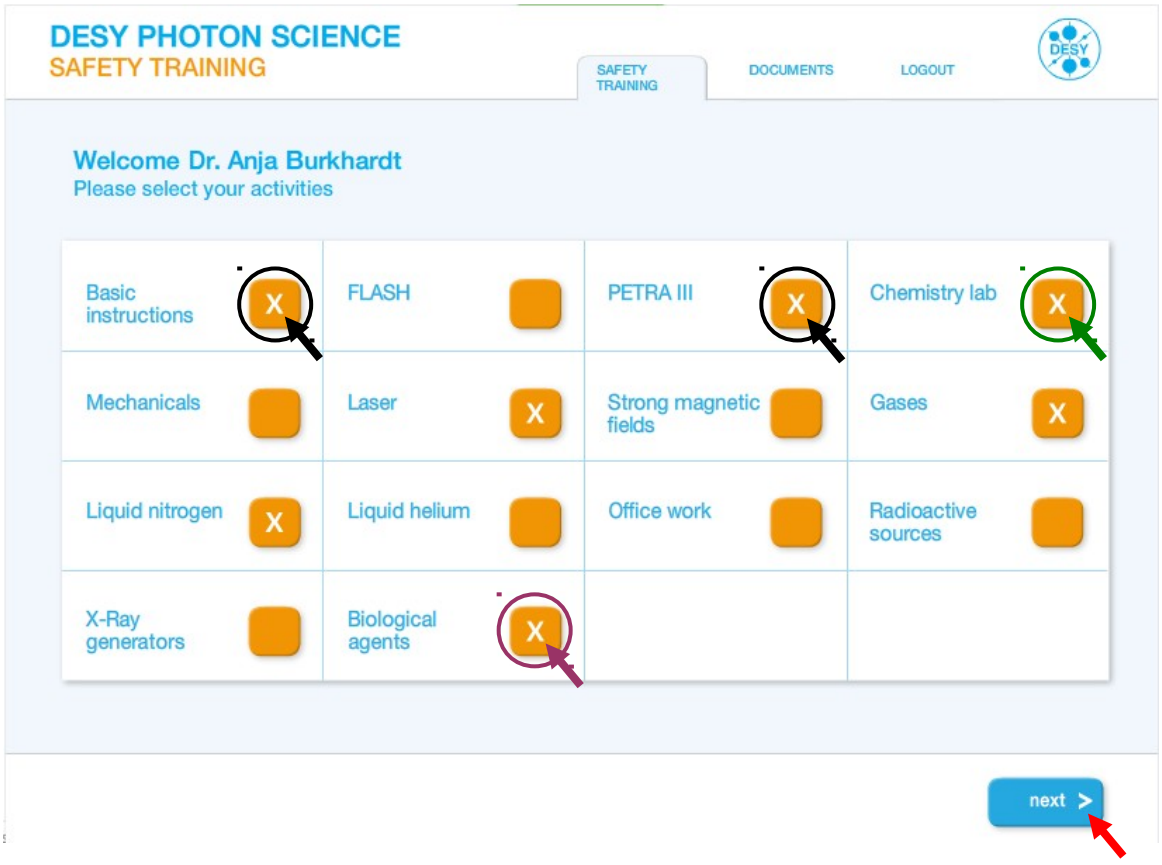

ACCELERATORS | PHOTON SCIENCE | PARTICLE PHYSICS
Deutsches Elektronen-Synchrotron
A Research Centre of the Helmholtz Association
DESY PHOTON SCIENCE »
DOOR HOME | ROLE SELECTION | CONTACT
DOOR
DESY Online Office for Research with Photons
GENERAL USER
» New Proposal
» Edit Proposals
» Declaration of Substances
» Register Participants
» Online Safety Training
» User Feedback
» User Infos
» Log off
REGISTRATION OF PARTICIPANTS
GENERAL INFORMATION
PI
Dr. Anja Burkhardt
Beamline
P11
Startdate
01-Oct-2015
Enddate
05-Oct-2015
EXPERIMENTERS AT THE BEAMLINE
Dr. Anja Burkhardt
SELECT
REMOVE
MAIN
SUBMIT
ADD EXPERIMENTER
LIST

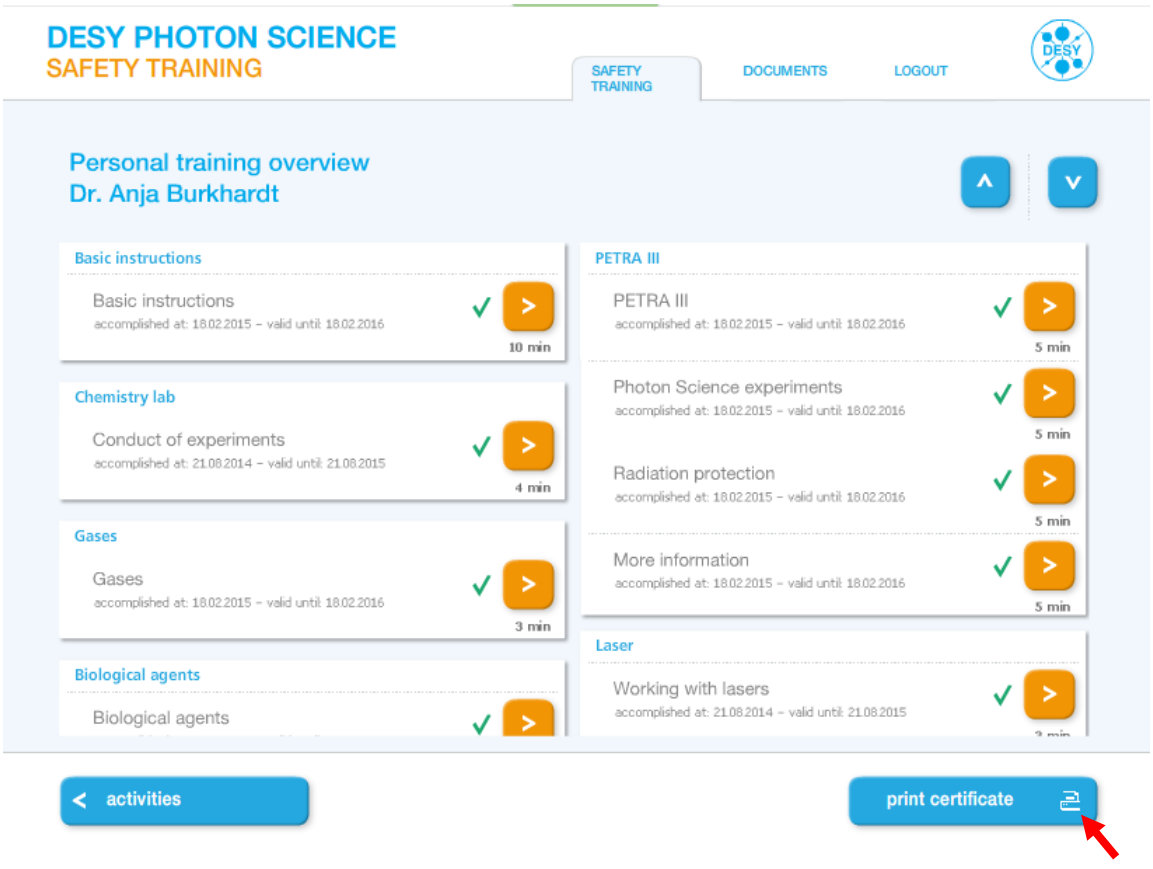
I.5. Online Safety Training



You are only allowed to perform your experiment at DESY if you obtained a valid and appropriate instruction. The online safety training consists of different modules and takes approx. 20 to 30 minutes, depending on your activities at P11. In order to get access to the beamline you need at least to pass the ‘Basic-Instructions’ and ‘PETRA III’ part.
Please select additional modules corresponding to your requirements:
- ‘Biological agents for access to the P11 user lab (S2 safety level, L047).
- ‘Liquid nitrogen’ for working with liquid nitrogen, e.g. flash-freezing of protein crystals
etc.

After you have completed the online safety training please send your signed safety certificate to the Photon Science Users' Office (preferably by fax +49 40 8998 4475).
Only after activating your signed safety certificate in the HASYLAB users’ office the successfully completed safety instructions will be valid.


DESY PHOTON SCIENCE
SAFETY TRAINING
SAFETY TRAINING
DOCUMENTS
LOGOUT
Welcome Dr. Anja Burkhardt
Please select your activities
Basic instructions
FLASH
PETRA III
Chemistry lab
Mechanicals
Laser
Strong magnetic fields
Gases
Liquid nitrogen
Liquid helium
Office work
Radioactive sources
X-Ray generators
Biological agents
next


DESY PHOTON SCIENCE
SAFETY TRAINING
SAFETY TRAINING
DOCUMENTS
LOGOUT
Personal training overview
Dr. Anja Burkhardt
Basic instructions
Basic instructions
accomplished at: 18.02.2015 – valid until: 18.02.2016
10 min
Chemistry lab
Conduct of experiments
accomplished at: 21.08.2014 – valid until: 21.08.2015
4 min
Gases
Gases
accomplished at: 18.02.2015 – valid until: 18.02.2016
3 min
Biological agents
Biological agents
PETRA III
PETRA III
accomplished at: 18.02.2015 – valid until: 18.02.2016
5 min
Photon Science experiments
accomplished at: 18.02.2015 – valid until: 18.02.2016
5 min
Radiation protection
accomplished at: 18.02.2015 – valid until: 18.02.2016
5 min
More information
accomplished at: 18.02.2015 – valid until: 18.02.2016
5 min
Laser
Working with lasers
accomplished at: 21.08.2014 – valid until: 21.08.2015
activities
print certificate

1.6. Requirements for biological samples (no protein crystals)

Working with biological agents categorized as biosafety level 2 is possible in the P11 laboratory. The online safety module "Biological agents" must be completed. All biological agents must be declared in DOOR: "Registration of biological agents". If you have special requirements (microscope, cell incubator, etc.) please contact the beamline staff beforehand. An second biosafety level 2 laboratory with additional equipment is available on request. Please contact the P11 beamline staff beforehand.

I.7. Accommodation

Accommodation is available at the DESY guesthouse. You can either send a request via DOOR or by contacting the guesthouse via http://guest-services.desy.de/hostel_in_hamburg/hostel%27s_info/.

Check-in time is from 14:00 onwards. Keys for the Hostel rooms may be collected from, or returned to, the Hostel Office (Mon-Fri 9:00 - 13:00) or the DESY Main Gatehouse, Notkestrasse (Mon-Fri 14:00 -9:00; weekends and public holidays: 24 h a day).

I.8. Dewar Shipping

If you are planning to ship your Dewar to P11 please get in touch with us via p11beamline@desy.de beforehand and provide us with the name of the shipping company and the tracking number.

a) General

1) Please empty the remaining liquid nitrogen completely, once the absorbent material within the Dewar is soaked. This will allow the shipment without declaring it as "Dangerous Goods". It is recommended to use cable ties to prevent unauthorized people from opening your Dewar.

2) Please schedule at least 3 working days between the day of dispatch and the start of your experiment at P11. Please arrange the delivery and pick-up of your shipments during standard working hours (Mo – Fr, 08:00 – 18:30). Otherwise we cannot guarantee a proper sample cooling as well as a secure arrival of your shipment at the beamline in time. On working days the P11 staff will take care of the Dewar and immediately refill it with liquid nitrogen once it has arrived at the beamline. Shipments will not be accepted on weekends and public holidays.

3) Please stick a label with “Priorität geforene Proben, PETRA III Bio Sample c/o DESY” on the outside of your package. In addition, we recommend to label your dry shipper with clearly visible safety and handling declarations, e.g. arrows pointing up or ‘Keep upright’ and ‘Do not drop’ or ‘Handle with care’.

b) Shipper Information

As a user, you are responsible for:
1) the declaration of the content of the Dewar (number and type of your samples e.g. ‘Cooling container with XXX frozen protein crystals for scientific experiments at receiver. Not dangerous.'), as well as for all the paperwork necessary related to the shipment of samples. Please note that an insufficiently or inaccurately described shipper content and packages containing samples which are not covered by IATA special provision A152 can cause a significant delay of the shipping procedure. This could lead to an interruption of the cooling chain and thawed, unfrozen samples.

2) following your courier's instructions and being aware of the policy of shipment from the country of origin, as well as eventual changes in the law.

3) all the **paperwork and costs** derived from the shipment of the Dewar from your home institution to DESY **as well as the return** from DESY to your home institution.

4) organizing the shipment from your home institute to DESY **and** from DESY back to your home institute

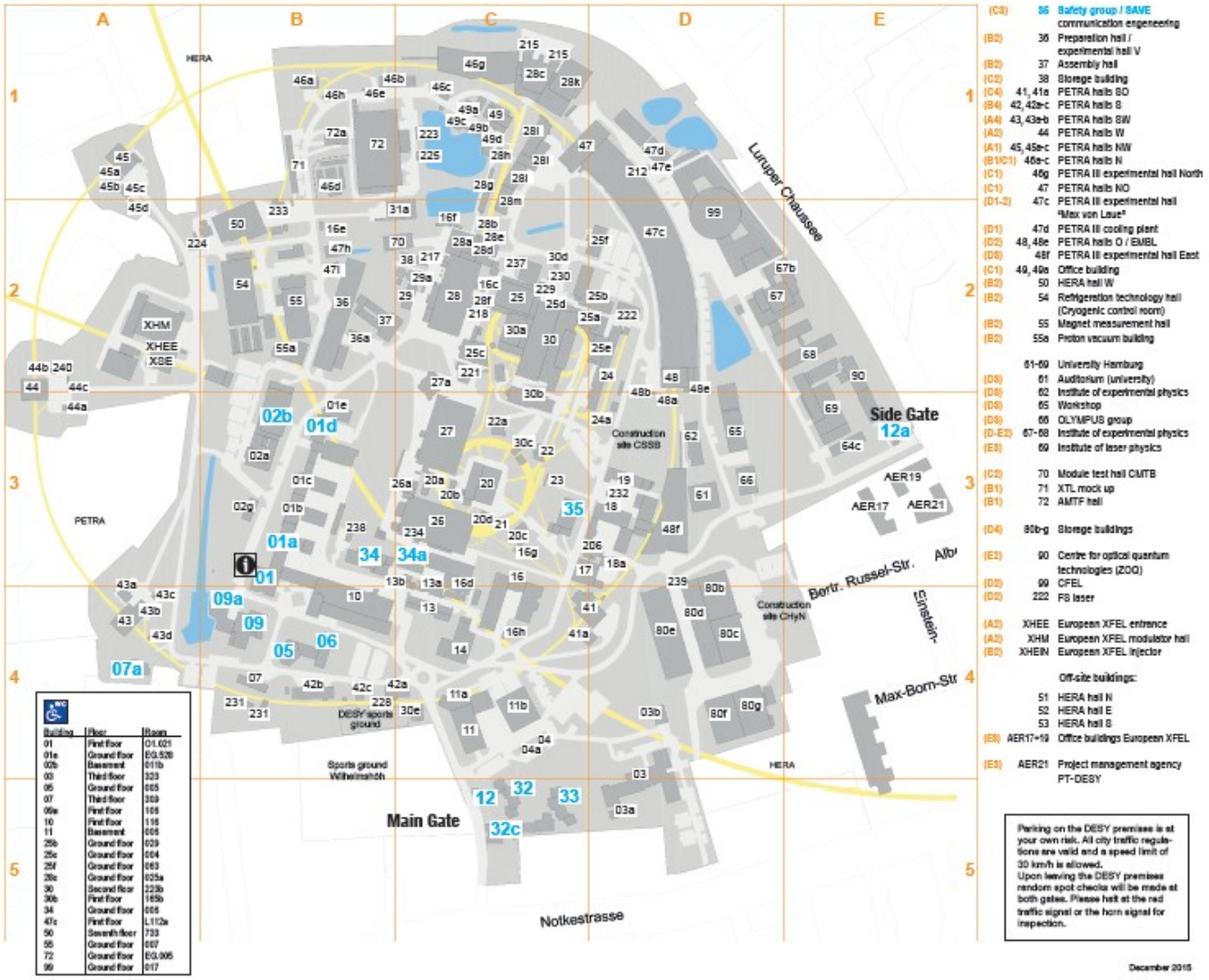
Shipping address:
PETRA III Bio Samples
CFEL Center for Free Electron Laser Science
c/o Deutsches Elektronen-Synchrotron DESY
Luruper Chaussee 149, Building 99, EG.001 Reception
22761 Hamburg
Germany
Phone: +49 40 8998 6666

For more details on the Dewar shipping to and from P11 please have a look at our webpage:
http://photon-science.desy.de/facilities/petra_iii/beamlines/p11_bio_imaging_and_diffraction/user_information/dewar_shipping/index_eng.html.

II. During Your Beamtime

II.1. Arrival at DESY

Detailed information on how to reach DESY can be found here:
http://photon-science.desy.de/about_us/how_to_reach/index_eng.html

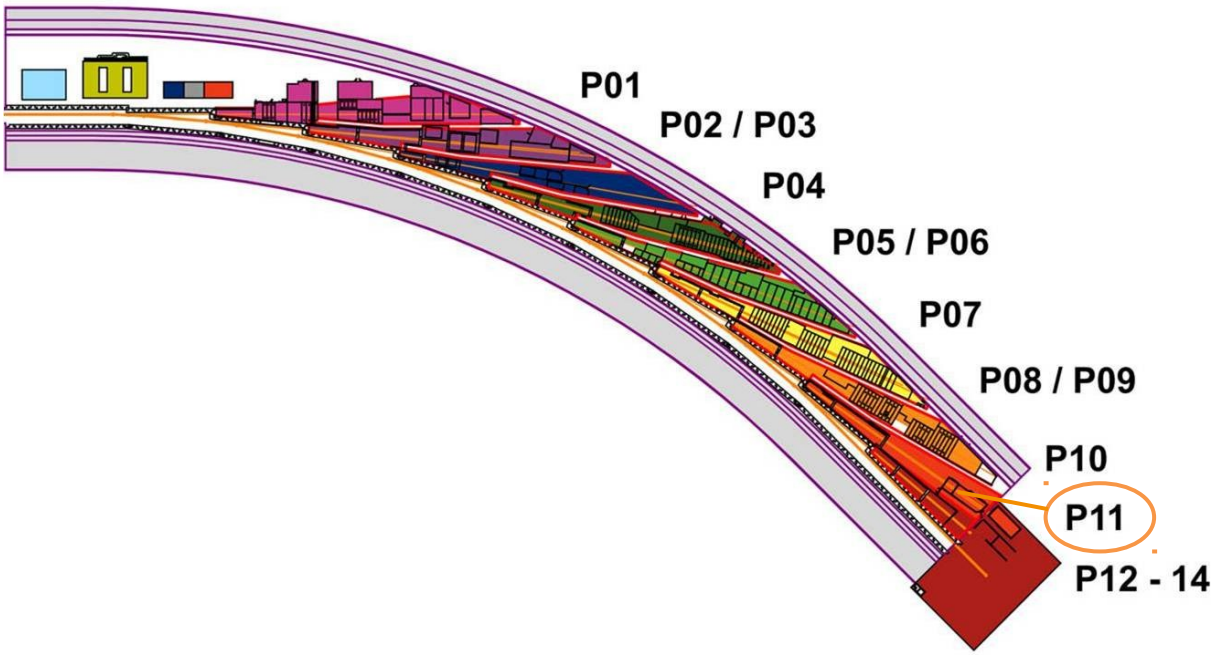


The DESY main entrance is located at Notkestrasse and is open at all times. The side entrance at the Luruper Chaussee is open for motorists from Monday till Friday, from 6:00 to 7:00, and closed on weekends. It is open for pedestrians and cyclists at all times.

Please get in touch with your local contact after your arrival on-site. You will be instructed at the P11 experimental station by your local contact. After the

instruction on-site you will receive the beam shutter permission.

PETRA III experimental hall from outside.



PETRA III experimental hall from inside.

II.2. Badges (DACHS cards)

At PETRA III all experimental areas as well as laboratories, mechanical workshops and the accelerators are secured by the control system DACHS (DESY ACcess Handling System). In order to get access to the P11 user lab and to operate the P11 beamline you will need a valid access card (DACHS card).

You will get your personalized DACHS card after successfully passing the safety instructions. Your DACHS card can be printed in building 6 / room 110 (during office hours, Mon-Thu 9:00 - 11:30 and 13:00 - 16:00, Fri 9:00 - 11:30 and 13:00 - 14:00) or at the gatekeepers at the DESY main entrance (Mon-Sun, 24 h). In exceptional cases you can obtain your DACHS card at the Photon Science Users' Office (PETRA III Experimental Hall ‘Max von Laue’, bldg. 47c / room L106).

If you have already obtained a DACHS card during an earlier visit to DESY please bring it with you, otherwise you will be charged the costs for a spare card.

The permission to work in the P11 user lab and to search the P11 experimental hutch must be granted by your local contact at the beamline. Afterwards you can use your DACHS card.

II.3. *Data Processing*

Data analysis during your experiment can be performed using computer **haspp11eval01.** You can login to this machine from the experimental PCs (**haspp11user02 - 04**) in the P11 control hutch via:

ssh p11user@haspp11eval01
The required password will be provided on-site by your local contact.

You can find your data here:
cd /gpfs/current

Various data processing and refinement software is available on **haspp11eval01**:
- BKchem
- CCP4
- COOT
- PHENIX
- PLATON
- xia2
- XDS
- SHELX
- Mosflm / iMosflm

- PyMOL
- Olex2
- OnDA
- CrystFEL

Additional information:
- The programs **ALBULA** and **adxv** may be used for visualization of your diffraction images.
- Text editors available on the P11 experimental PCs are e.g. **Nedit** or **Emacs**.

a) Automatic Processing with XDSAPP

A data collection strategy is automatically calculated for each screening experiment via **mosflm**.
You can access the the generated .log file via:
cd /gpfs/current/processed/DataSet/DataSet_screening_X/strategy/mosflm.log

In order to get the necessary information (optimum rotation rage for native and anomalous data collection) please type:
grep -A 2 "*Optimum*" *mosflm.log*

Each data set collected at P11 will be automatically processed using the program package **XDSAPP**.

You can access your results from automatic data processing via:
cd /gpfs/current/processed/DataSet/DataSet_X/
There you will find 2 folders:
1) *pre*: partial data set processed at limited resolution range, allows fast feedback on your crystal and its diffraction properties.
2) *full*: complete data set (all frames collected) processed at the maximum resolution range

b) Manual Processing with XDSAPP

XDSAPP (v0.21) is a GUI for the XDS package developed by the Helmholtz Centre Berlin. The input file is optimized for the P11 beamlime parameters.

Please go to your data folder and type the command *xdsapp*, which will open the XDSAPP GUI. Processing outputs are stored in the subfolder 'xdsapp'.

Select Pilatus6M as detector type and your single or multiple data sets for analysis.

For further details please check the primary literature for XDSAPP: M. Krug *et al*., *J. Appl. Cryst*. (2012), **45**, 568-572. http://scripts.iucr.org/cgi-bin/paper?S0021889812011715

If the automatic procedure fails you can also manually process your data.

c) Manual Processing with XDS (command line)

For manual processing with **XDS** you may proceed as follows:
1) Go to your data folder
2) After you have modified the XDS.INP file according to your data collection parameters (detector distance, oscillation range, data range, etc.) you can start the program **XDS** with *xds_par*

II.4. Data Backup

a) During Your Experiment

You can backup your data to your own external hard disk via an USB 2.0/3.0 or Firewire connection. Supported formats are NTFS, ext4 or ext3.

Please connect your external disk to computer **haspp11user01** which is located next to the printer in the P11 control hutch. Your hard disk will be automatically mounted on this computer. You can copy your data using the python script **rsync_command.sh** which is available in via /home/p11user on **haspp11user01**.

To avoid waiting time, please start the backup as soon as possible after your initial experiments.

b) After Your Experiment

Once you have finished your experiment access to the local disks at P11 will no longer be granted.
You can download your data earliest 3 days after your beamtime via https://gamma-portal.desy.de
All participants registered for the experiment via DOOR will have access to the data and are authorized to download it from the gamma portal.

To download your data you need to login to the gamma portal using your DOOR username. A detailed documentation on the DESY gamma portal is given here: https://confluence.desy.de/display/ASAP3/The+Gamma+Portal

III. After Your Experiment

After your beamtime is over you are kindly asked to get in touch with your local contact.

Please remove your waste and dispose it properly.

Please take or send back all your samples (chemicals, Dewars, equipment, etc.) to your home institution.

Please keep your DACHS card for future experiments at DESY Photon Science.

Please do not forget to collect and pay the bill(s) of the DESY hostel (or alternative accommodation).

In order to improve our service at P11 we rely on your comments and suggestions. Therefore we would like to ask you to submit a "Users' feedback" form via DOOR. In addition, you are kindly asked to submit an experimental report for each beamtime in DOOR. Please note that the experimental report is mandatory for proposal users and plays a crucial role for the evaluation of your future proposals at P11.