# 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 <u>https://door.desy.de/door/index.php</u> 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 <u>photon-science@desy.de</u>.

d) Submit the completed form

DESY	ADDELERATORS   PHOTON BOLENCE   PARTICLE PHYSICS Decision Environment Application - A Reserve Carlor of a method association	DESY P	HOTON SCIENCE »
	DOOR HOME CONTACT		
DOOR DESY Online Office for Research with P			
HOME New User			
Lost Password     Registered Liner	Proposal Submission FLASH	01-Apr-2015	
- regissite cas	 The Call for Proposals for FLASH experiments during the period January to June 2016 is open. Due to oldi constructions related to the PETRA III Extension no regular beamtime vill be available at PETRA III from 3 February 2014 until 27	April 2015.	
	Weisome to DOOR, the DESY Online Office for Research with Protons. After registration, you may use this system to submit research proposals or beamtime applications, and to complete all administrative steps re- reintoursement, registration of publications). Please do not hesitate to contact us in case you have further questions or if you encounter any problems using DOOR.	pulred prior and after your experiment (e.g. online safely training, submission of declaration of substances, registration of participants, travel	
	Registered DORR user Log on using your DORR user name and password or your Umbretia oredentass. Forgothen gesevoid If you on not remember your DOOR user name and/or password, your log on information will be sent to your previously registered e-mail accress.	New DOOR user To coate a DOOR user name and passesions, please register here. Users with an existing Uniterial account might final log on at Uniterial Index Or you might set up an Uniterial account before registering Nete	

6		ACCELERATORS PHOTON SCIENCE PARTICLE PHYSICS Deutone Systeme Systematic another and the Sector and Sector S		DESY PHOTON SCIENCE >>
P	SY	DOOR HOME CONTACT		
DOC DESY Onlin	)R ne Office for Research with Phot			
HOME > New us			DOOR USER REGISTRATION	
Lost Pa Regist	issword ered User		REGISTER NEW DOOR USER	
		In odde to be able to submit proposals for the DESY light sources, you must for continuation. DOOR user name (*) Passevord (*) Continn password (*) E-mail address (*) Institute (*) Department Address	st register to DOOR. Please enter your desired user name, your e-mail address an	o other required details in the form below. After submitting the form, an e-mail will be send to the given address for SSLECT
			ů	REPORT INCORRECT ADDRESS
			APPETHENT TO RESPONSE DATA HERITATION DESCRIPTION DEPENDENT	NO TELLE AU AUDITURE IN
		1. Jagree that my personal data are stored in the DOOR datase systems).     2. I assure that all my research activities at DESY Photon Science     3. I confirm that I have read and accept the Terms and Conditions 1	e and thrwarded to the central person associate at DESY for memal operational an are conducted exclusively for peaceful purposes and in accordance with the gene of Commercial User Access (applicable to commercial users) or Terms and Cond (*) these Twicks are mandatory	o ammiatrative purposes, in hocessary, the data may be triviarided to other DESY information systems (e.g. access control arally accepted rules for good scientific practice, attions for Non-Proprietary User Access (applicable to non-commercial scientific users).
		INSTITUTES	Salari Carca	
max	planck	institutio	SEARCH CLEAR	
	Institute/Depart	tment	Country	
Select	Max-Planck-Ges	elischaft	Germany	
Select	Max-Planck-Ges Max Planck Instit Archaeology and	elischaft ute for Evolutionary Anthropology Max Planck Weizm Anthropology	Germany ann Center for integrative	
Select	Universitaet Ham Max Planck Grou	iburg p for Structural Dynamics (CFEL)	Germany	
		I DON'T FIND MY INSTITUTE CLOS	E	

### *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.

DESY	ACCELERATORS   PHOTON SCIENCE   PARTICLE PHYSICS Deutsches ElektronenSynchoton A Research Centre of the Heinholtz Association	DESY PHOTON SCIENCE »
DOOR DESY Online Office for Research with Ph	notons	
GENERAL USER		
» New Proposal	GEN	ERAL USER
» Edit Proposals	Full name	Dr. Anja Burkhardt
» Declaration of Substances	DOOR user name	burkhardt
Register Participants	Umbrella user name	DOOR account not linked with an Umbrella account
» Online Safety Training (requires Flash)		
» User Feedback	nu	
» Experimental Reports	PROPOSALS - BEAMTIME APPLIC	ATIONS - EXPERIMENT SPECIFICATIONS
<ul> <li>&gt;&gt; User Infos</li> <li>&gt;&gt; Log off</li> </ul>	Submit a new proposal New proposals may be submitted here. If you leave DOOR before completing the submission, your entries are saved and may be edited and completed later (see below)	Follow-up applications for beamtime for a PETRA III long-term project If you have a valid PETRA III long-term project, you may apply for beamtime here Please note: Applications may be submitted only during valid for long-term projects
	2004).	Confirm FLASH application for beamtime
	Edit/Delete a partially completed proposal If you have not completed the submission procedure (see above), you may edit/complete/delete your entries here. Once a proposal is submitted, it cannot be	If your FLASH proposal has been accepted, please confirm your application for beamtime here.
	modified or deleted by yourself. In this case you need to contact the users office.	Submission of experiment specifications for additional proposal types at PETRA IIVFLASH
<	View your proposal(s) Proposer or co-proposers may view the pdf-version of their proposal(s).	Submission of experiment specification is required for - Commercial/Industrial proposals - NFFA proposals - Cooperation projects with MPG and Helmholtz Groups Experiment specifications related to one of these proposal types can be submitted throughout the year.

<b>SY</b>	ACCELERATORS   PHOTON SCIENCE   PARTICLE PHYSICS Detaches Electron-Synchron A Research Centre of the Herindits Association		DESY PHOTON S
	DOOR HOME   ROLE SELECTION   CONTACT		
	and the second		
JR			
ne Office for Research with Photo	R - Charles and the second second second		
SEARCH			
ation of Substances		APPLICATION FOR BEAMTIME	
Chemistry Laboratory		DEMILDED DEAMI INC ARELD ON DEAMI INCO. DETDA HI DEAMI INCO.	
er Participants	Experimental station assigned	PETRA III: P11	
er your Publications	Beamline setup/instrument (*)	Crystallography (1-axis goniostat)	
		CENEDRI INCODIRATION	
	Number of chiffs (Sh) renulised (4)		
	Photon energylenergies (*)		
	Ream and size on sample (*)		
	rang note ()	O 40 bunches O 60 bunches O multi bunches I any	
	Destingent start data	PREFERRED DATES (FOR BEAMTIME BETWEEN JULY AND DECEMBER 2016)	
		SELECT DEVICES	
		DETECTORS (*)	
	Pilatus 6M (2463*2527 pixels, 172x172µm*)	O Yes O No	
	Vortex EM SI drift detector	C Yes 🖲 No	
		EQUIPMENT (*)	
	Sample changing robot (unl-puck format)	Ves 🔍 No	
		ACCESS TO DESY NANOLAB	
	DESY NanoLab access (*)	- Select one -	
		OPTIONAL ADDITIONAL MESSAGE	
		(*) these fields are mandatory.	
		MAIN SAVE	
		MAIN SAVE	

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

# I.3. Declaration of Substances

DESY	ACCELERATORS P Deutsches Elektronen-S A Research Centre of th	HOTON SCIENCE PARTICLE PHYSIC ynchrotron w Helmholtz Association	cs			DESY PHOTON SCIEN
	DOOR HOME R	LE SELECTION CONTACT				
DOOR SY Online Office for Research with Pho	tons		28			
ENERAL USER			CEN			
New Proposal			GEN	Chal USEN		
dit Proposals	Full name			Dr. Anja Burkhardt		
eclaration of Substances	DOOR us	ername		burkhardt		
egister Participants	Umbrella	user name		DOOR account not linked	with an Umbrella account	
nline Satety Iraining (requires Flash)						
ser Feedback				ATIONS EVERIMENT SPECIE	CATIONS	
perimental Reports			PROPUBALO - BEAMTIME APPLIG	ATTONO - CAPENIMENT SPECIFI	CALIDINA	
ser Infos og off	Submit a New pro submiss	n <b>ew proposal</b> posals may be submitted here. If y on, your entries are saved and m	you leave DOOR before completing the ay be edited and completed later (see	Follow-up applications the follow of the follow of the following of the fo	for beamtime for a PETRA III k A III long-term project, you may s may be submitted only during	ong-term project apply for beamtime here. calls for long-term projects!
	Edit/Del If you ha edit/com	ete a partially completed propos ve not completed the submission plete/delete your entries here. On	al procedure (see above), you may ce a proposal is submitted, it cannot be	Confirm FLASH applica If your FLASH proposal I beamtime here.	tion for beamtime nas been accepted, please con	firm your application for
	modified View yo Propose	or deleted by yourself. In this cas <b>IF proposal(s)</b> or co-proposers may view the po	e you need to contact the <b>users office</b> . If-version of their proposal(s).	Submission of experim III/FLASH Submission of experime - Commercial/Industrial - NFFA proposals - Cooperation projects y	ent specifications for addition nt specification is required for proposals with MPG and Helmholtz Group	al proposal types at PETRA
				Experiment specification throughout the year.	s related to one of these propo	sal types can be submitted
NOR Indue Office for Research with Photons AL USER Proposal			DECLARATION OF S	UBSTANCES		
Proposals			LIST OF SCHEDULED SHIFTS W	THOUT DECLARATION		
ster Participants		Start	End	Proposal	Beamline	Shifts
Safety Training	lectaration	01-Oct-2015 17-Sep-2015	05-Oct-2015 21-Sep-2015	C-20010001	P11	12
Feedback	lectaration	14-Aug-2015	17-Aug-2015	H-20010012	P11	9
	eclaration	27-Apr-2015	01-May-2015	C-20010001	P11	9
N	io declarations so far!		DECLARATION OF SUBSTANCES FO	R CURRENT BEAMTIMES		
			LIST OF SCHEDULED SHIFTS	WITH DECLARATION		
Y	ou oo not have any scheduled sh	ns wan declaration!				
			MAIN MANAGE FAVO	NTE 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.

EntrySafety CategoryProtein crystalsHarmless, non-toxic, non-infectiousProtein crystalsInfectious. These are proteins which need to be classified as a<br/>biological agent according to the BioStoffV e.g. agents<br/>associated with transmissible spongiform encephalopathy,<br/>such as prions.Protein crystalsToxic

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).

DESY	ACCELERATORS   PHOTON SCIENCE   PAR Deutsches Siekizone-Synchrotron A Research Certier of the Heimholtz Association	TICLE PHYSICS							DESY PHOTON SCIENCE )
	DOOR HOME   ROLE SELECTION   CONTA	AGT							
DOOR DESY Online Office for Research with Phot	uns								
GENERAL USER  New Proposal  Edit Proposals  Dealerstein of Evidences				SAI	ETY ASPECTS FOR BEAMTI (01-0CT-2015 TO 05	ME AT BEAMLINE P11 -oct-2015)			
Register Participants	DECLARATIO	N OF SUBSTANCES	REGISTRATIO	N FOR CHEMISTR	I LABORATORY	BIO SAFETY REGISTRATI	DN	LASER SAFETY REGISTRATION	
Online Safety Training									
User Feedback					GENERAL INFORM	IATION			
User infos	Project Number				C-20010001				
- Log on	Principal investigator				Dr. Anja Burkhardt				
	Project Leader								
	Beamline				P11				
	Standate				01-001-2015				
	Chouse				00-00-2010				
					REGISTRATION D	ATES			
	Startdate (*)				01/10/2015	SELECT	(dd/mm/yyyy)		
	Enddate (*)				05/10/2015	SELECT	(dd/mm/yyyy)		
			SUBSTAI	NCES (SELECT AL	SUBSTANCES TO BE USED AT THI	E EXPERIMENT, EXCEPT BIOLOGICAL AGEN	TS) (*)		
	Substance	Protein crystals	SELECT	REMOVE		Amount (and rem	arks)	50 crystals	
	Substance		SELECT	REMOVE		Amount (and rem	iariks)		
	Substance		SELE	REMOVE		Amount (and rem	iarks)		
	Substance		SELECT	REMOVE		Amount (and rem	arks)		
	Substance		SELECT	REMOVE		Amount (and rem	arks)		
	Substance		SELECT	REMOVE		Amount (and rem	arks)		
	Substance		SELECT	REMOVE		Amount (and rem	arks)		

				EDECIAL	CONDEMENTS		
		Use of chemistry laboratory (*)		- Select one -	-		
		Use of biological agents (at beamline or in S1 bio la	(boratory) (*)	- Select one -	÷.		
		Use of gases (*)		- Select one -	-		
		Use of own lasers (*)		- Select one -	-		
			IIPI DAD SAFETY CON	CEPT (DETAILS ON EXPERIMENTAL SET	IP INCLUDING DIMENSIONS SL	ING POINTS FTC. FOR TRANSPORT)	
		Safety concept				SELECT REMOVE	
			LIST OF	HAZARDOUS EQUIPMENT (E.G. OVENS,	PRESSURE CELLS) TO BE USED	AT THE EXPERIMENT	
		This is a complete list of all substance. We have	the set of all based on a second The second	nat comellar to European directions	a shadarde and is analysis in t	na datu I bini manifin falinu ita ma dari afiti ana dari	e and in latera we as workers. Lineally alreader
		DESY for any damage or injury resulting from my fa	ties and or all nazaroous equipment. The equipm fure to follow the safety procedures.	nenc complies to European directives a	nu stanuaros ano is controlled r	regularity: Lonio myself to tollow the required safety procedure	s and to inform my co-workers. I nereby absone
		Accept (*)					
				(*) these fiel	de are mandatory.		
				MAIN SUBMIT	ADD SUBSTANCE LIST		
HELMHOLT	t IAFT						© 2013 Deutsches Elektronen-Sunchrotron
		ADD SUBSTANCE					
protein	crystals		SEARCH CLEAR				
	Substance	Aggregate	CAS no.				
Select	Protein crystals	solid/piece(s)	_				
Colort	Diretale encials lef	colldisions(c)					
Jeleul	Protein drystals Int.	autorpiece(a)	_				
	If you cannot find a	substance, click here to ad	d it manually!				
	-	-	-				
		CANCEL					

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.

		DEGLARATI	ON OF SUBSTANCES			
		LIST OF SCHEDULED	HIFTS WITHOUT DECLARATION			
	start	End	Proposal	Beamiline	Shi	
Declaration	01-Oct-2015	05-Oct-2015	C-20010001	P11	12	
Declaration	17-Sep-2015	21-Sep-2015	H-20010012	P11	12	
Declaration	14-Aug-2015	17-Aug-2015	H-20010012	P11	9	
Declaration	27-Apr-2015	01-May-2015	C-20010001	P11	9	
DECLARATION OF SUBSTANCES FOR CURRENT BEANTIMES						
No declarations so far!						
		LIST OF SCHEDULE	I SHIFTS WITH DECLARATION			
You do not have any scheduled	d shifts with declaration!					

DESY	ACCELERATORS   PHOTON SCIENCE   PART DeJushes Elektronen-Synchrotion A Research Certine of the Heimholiz Association	ICLE PHYSICS			DESY PHOTON SCIEN
	DOOR HOME   ROLE SELECTION   CONTA	CT			
DOOR ESY Online Office for Research with Phy	otons				
ENERAL USER New Proposal Edit Proposals			SAFETY ASPECTS FOR BEAMI (01-OCT-2015 TO 0	IME AT BEAMLINE P11 S-OCT-2015)	
Declaration of Substances     Register Participants	DECLARATIO	N OF SUBSTANCES	REGISTRATION FOR CHEMISTRY LABORATORY	BIO SAFETY REGISTRATION	LASER SAFETY REGISTRATION
Online Safety Training     User Feedback     User Infos	•	SELECT SU	BSTANCES FROM YOUR FAVORITES LIST TO ADD THEM TO THE DECLARATI	ON OF SUBSTANCES. MORE SUBSTANCES CAN BE ADDED IN THE NEXT STE	Ρ.
Log off			LIST OF SUBSTANCES MAR	KED AS FAVORITES	
	Selection	Substance	Symbol/Formula	CAS no.	Data sheet
	Select	Acetic acid	снасоон	64-19-7	view
	Select	Hydrochloric acld	HCI	7647-01-0	vlew
	Select	Protein crystals		-	-
	Select	Sodium hydroxide	NaOH	1310-73-2	view
			MAIN PROCEED WITH DECLARATION	MANAGE FAVORITES LIST	

# 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.

DESY	ACCELERATORS PHO TON SCIENCE PARTICLE PHYSICS Deutsches Elektronen-Synchrotron A Research Centre of the Helmholtz Association	DESY PHOTON SCIENCI
	DOOR HOME ROLE SELECTION CONTACT	
DOOR DESY Online Office for Research with Phot		
GENERAL USER		
» New Proposal	GENI	ERAL USER
» Edit Proposals	Full name	Dr. Anja Burkhardt
» Declaration of Substances	DOOR user name	burkhardt
» Register Participants	Umbrella user name	DOOR account not linked with an Umbrella account
» Online Safety Training (re, tes Flash)		
» User Feedback		
» Experimental Reports	PROPOSALS - BEAMTIME APPLICA	ATIONS - EXPERIMENT SPECIFICATIONS
» User Infos	Submit a new proposal	Follow-up applications for beamtime for a PETRA III long-term project
» Log off	New proposals may be submitted here. If you leave DOOR before completing the	If you have a valid PETRA III long-term project, you may apply for beamtime here.
	submission, your entries are saved and may be edited and completed later (see	Please note: Applications may be submitted only during calls for long-term projects!
	below).	Confirm FLASH application for beamtime
	Edit/Delete a partially completed proposal	If your FLASH proposal has been accepted, please confirm your application for
	If you have not completed the submission procedure (see above), you may	beamtime here.
	edit/complete/delete your entries here. Once a proposal is submitted, it cannot be	
	modified or deleted by yourself. In this case you need to contact the users office.	Submission of experiment specifications for additional proposal types at PETRA III/FLASH
	View your proposal(s)	Submission of experiment specification is required for
	Proposer or co-proposers may view the pdf-version of their proposal(s).	- Commercial/Industrial proposals
		- NFFA proposals
		- Cooperation projects with MPG and Helmholtz Groups
		Experiment specifications related to one of these proposal types can be submitted throughout the year.

ACCELERATORS | PHOTON SCIENCE | PARTICLE PHYSICS Delates Eletrone-Synchronen A Reserve Centre of the Hermitelia Association DESY PHOTON SCIENCE » DESY DOOR HOME | ROLE SELECTION | CONTACT DOOR DESY Online Offic USY Unite Unite for Hoseer CENERAL USER \* New Proposal \* Exit Proposals \* Declaration of Substances \* Register Participants \* Online Safety Training \* User Feedback \* User intos \* Log of REGISTRATION OF PARTICIPANTS LIST OF SCHEDULED SHIFTS WITHOUT REGISTRATIONS start 01-Oct-2015 17-Sep-2015 14-Aug-2015 27-Apr-2015 End 05-Oct-2015 21-Sep-2015 17-Aug-2015 01-May-2015 Proposal C-20010001 H-20010012 H-20010012 C-20010001 Beamline P11 P11 P11 P11 P11 Shifts 12 12 9 REGISTRATIONS OF PARTICIPANTS FOR CURRENT BEAMTIMES

No registrations so far!



#### ADDELERATORS | PHOTON SCIENCE | PARTICLE PHYSICS Deutsches Elektronen-Synchrotron A Research Centre of the Hembolic Association

DOOR H	OME   ROLE SELECTION   CONTACT						
Research with Photons							
		REGISTRATION OF PARTICIPANTS	S				
20005	GENERAL INFORMATION						
nts	PI	Dr. Anja Burkhardt					
	Beamline	P11					
	Startdate	01-Dct-2015					
	Enddate	05-Oct-2015					
		EXPERIMENTERS AT THE BEAMLINE					
		Dr. Anja Burkhardt	SELECT	REMOVE			
			SELECT	REMOVE			
			eci	REMOVE			
				THE REAL PROPERTY OF THE PROPE			
			SELECI	REMOVE			
			SELECT	REMOVE			

DESY PHOTON SCIENCE »

# I.5. Online Safety Training

DESY	ACCELERATORS PHOTON SCIENCE PARTICLE PHYSICS Dadaschae Elektronen Synchrotion A Research Centre of the Helmholtz Association	DESY PHOTON SCIEN	
	DOOR HOME ROLE SELECTION CONTACT		
DOOR ESY Online Office for Research with P	hotons		
GENERAL USER	-		
» New Proposal	GEN	GENERAL USER	
» Edit Proposals	Full name	Dr. Anja Burkhardt	
Declaration of Substances	DOOR user name	burkhardt	
Register Participants	Umbrella user name	DOOR account not linked with an Umbrella account	
» Online Safety Training (requires Flash	)		
» User Feedback			
» Experimental Reports	PROPOSALS - BEAMTIME APPLICATIONS - EXPERIMENT SPECIFICATIONS		
» User Infos	Submit a new proposal	Follow-up applications for beamtime for a PETRA III long-term project	
Log off	New proposals may be submitted here. If you leave DOOR before completing the	If you have a valid PETRA III long-term project, you may apply for beamtime here.	
	submission, your entries are saved and may be edited and completed later (see	Please note: Applications may be submitted only during calls for long-term projects!	
	below).	Confirm El ACH ann linguine des baserations	
	Edit/Delete a partially completed proposal	If your FLASH application for beamtime	
	If you have not completed the submission procedure (see above), you may	beamtime here.	
	edit/complete/delete your entries here. Once a proposal is submitted, it cannot be		
	modified or deleted by yourself. In this case you need to contact the users office.	Submission of experiment specifications for additional proposal types at PETRA III/FLASH	
	View your proposal(s)	Submission of experiment specification is required for	
	Proposer or co-proposers may view the pdf-version of their proposal(s).	- Commercial/Industrial proposals	
		- NFFA proposals	
		<ul> <li>Cooperation projects with MPG and Helmholtz Groups</li> </ul>	
		Experiment excellence related to any of these proposal types can be submitted	

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.



### *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 <u>http://guest-services.desy.de/hostel\_in\_hamburg/hostel%27s\_info/</u>.

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.

### <u>a) General</u>

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: <u>http://photon-science.desy.de/about\_us/how\_to\_reach/index\_eng.html</u>



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 **mosfim**.

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" mosfim.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. <u>http://scripts.iucr.org/cgi-bin/paper?</u> <u>S0021889812011715</u>

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 **haspplluser01** 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 **haspplluser01**.

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 <u>https://gamma-portal.desy.de</u>

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: <u>https://confluence.desy.de/display/ASAP3/The+Gamma+Portal</u>

# **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.