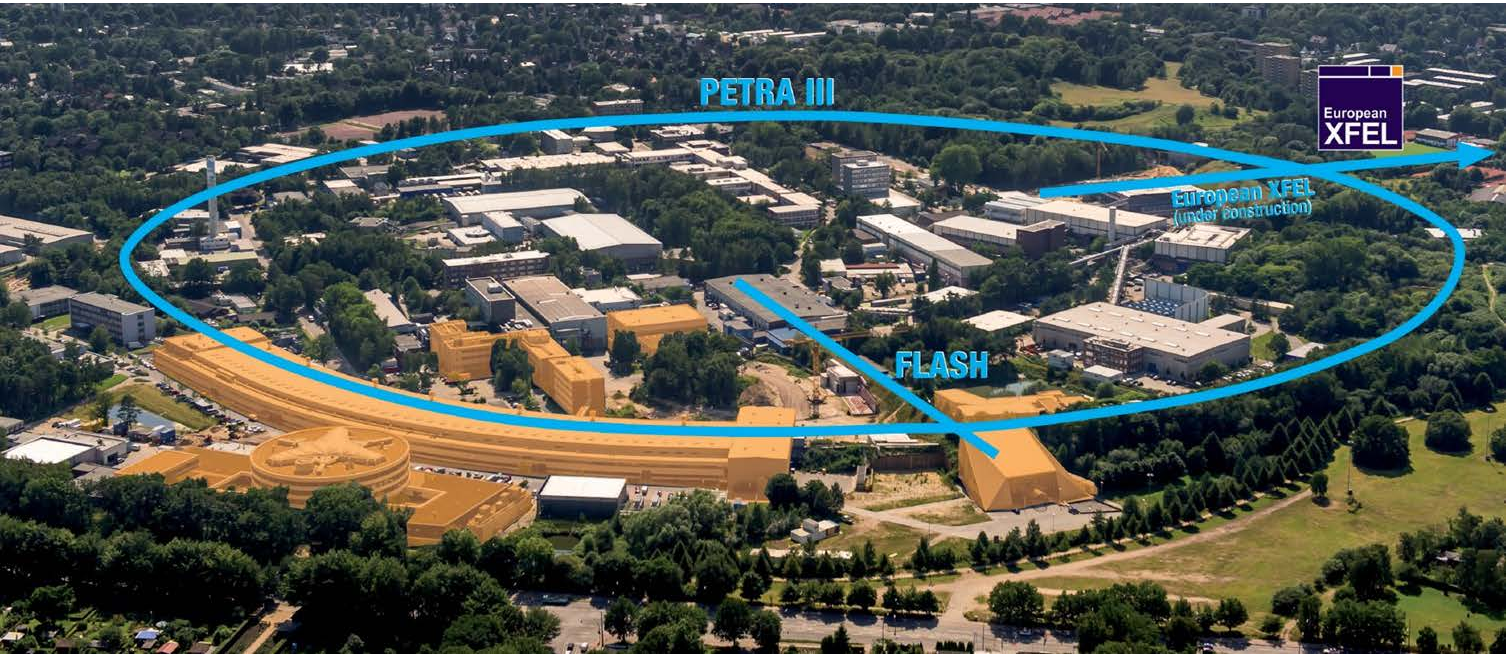
DESY Photon Science Facility Overview

USER OFFICE workshop – Three-Way Meeting



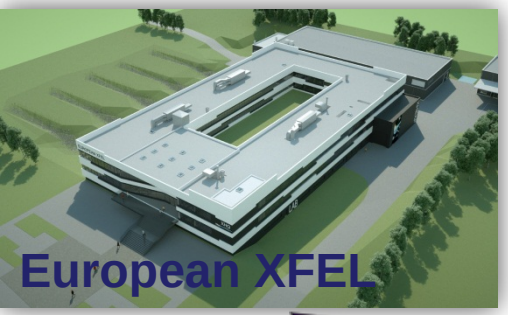
Daniela Unger

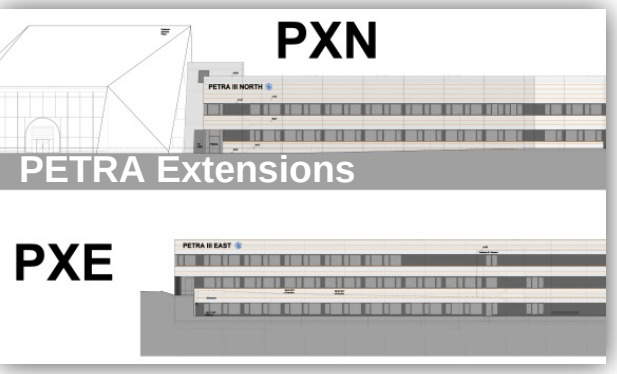
DESY Photon Science - Facility Overview
Three-Way Meeting
Argonne, July 31, 2013

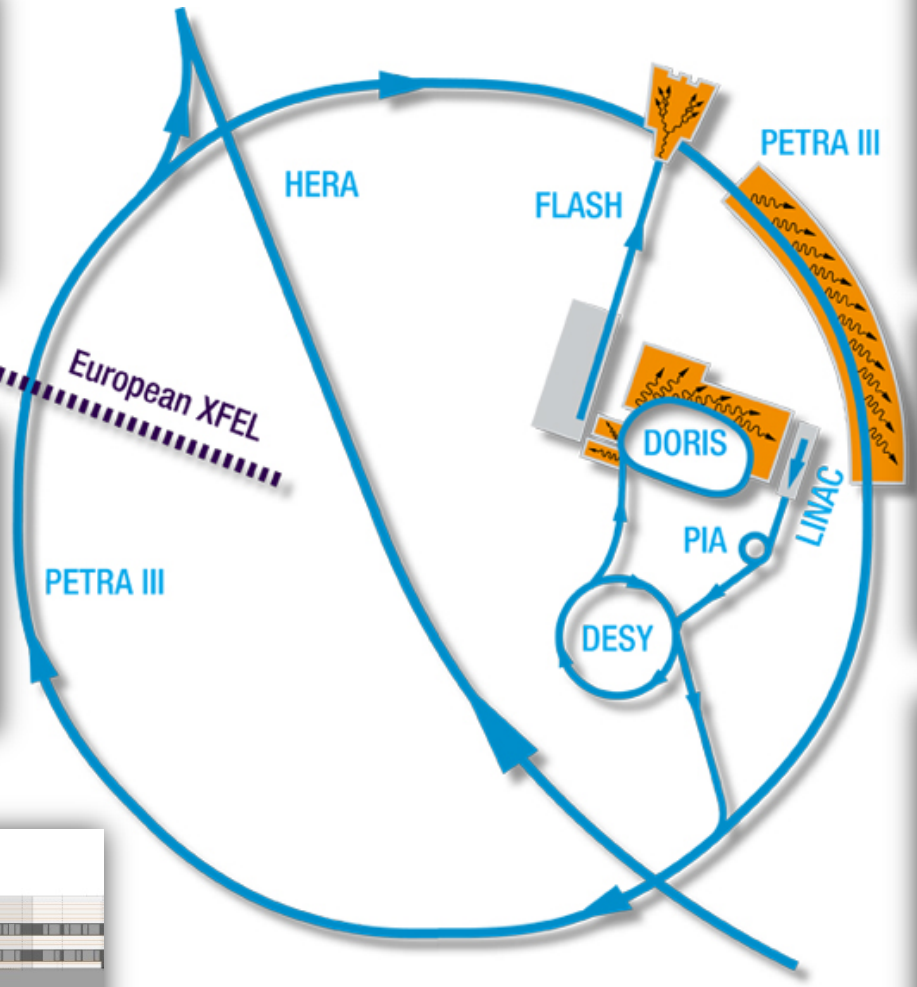
HELMHOLTZ ASSOCIATION

DESY

Photon Facilities at DESY





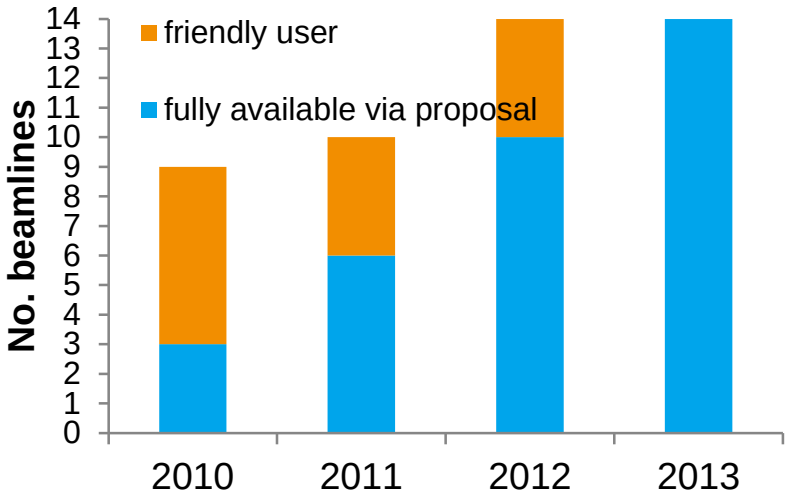


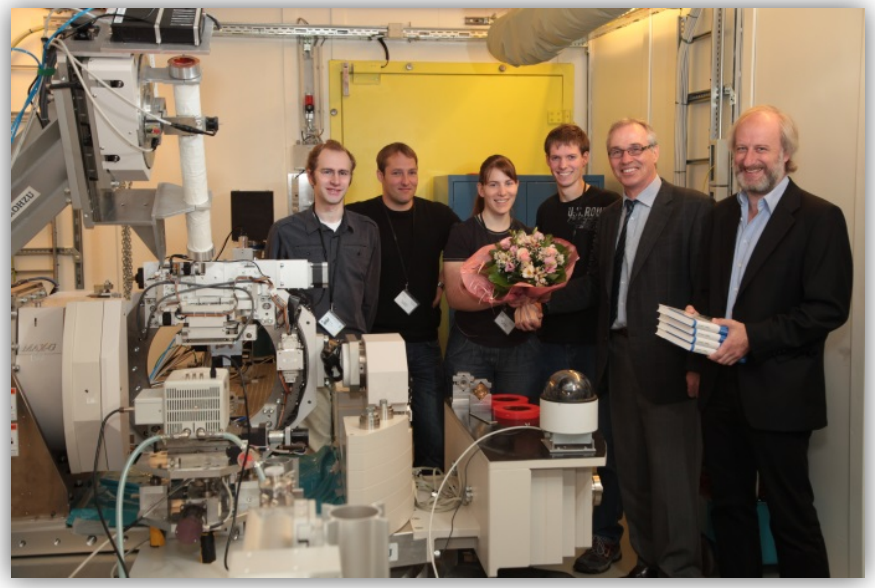
PETRA III - History

- PETRA accelerator originally served for particle physics experiments, then as a pre-accelerator for the large HERA facility
- After the shutdown of HERA in 2007, the 2.3-kilometre-long ring accelerator was refurbished and nearly 300 m completely rebuilt including a new experimental hall

PETRA III - History

- PETRA III took up operation in 2009
  - April 2009: first stable beam in the ring in April 2009
  - 12 Oct 2009: first users experiment at beamline P08.
  - 3 Sep 2010: first official user access,
  - regular operation started with 3 beamlines
  - 14 beamlines operational since 2012

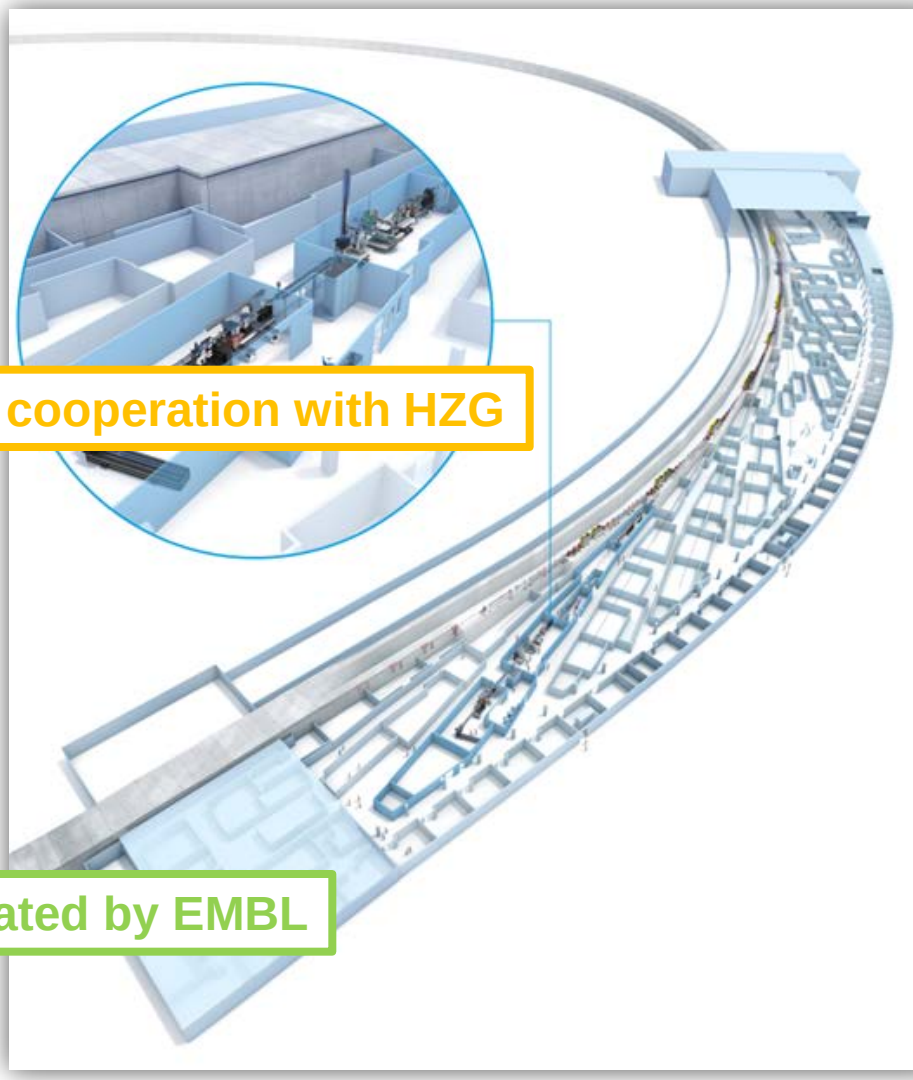




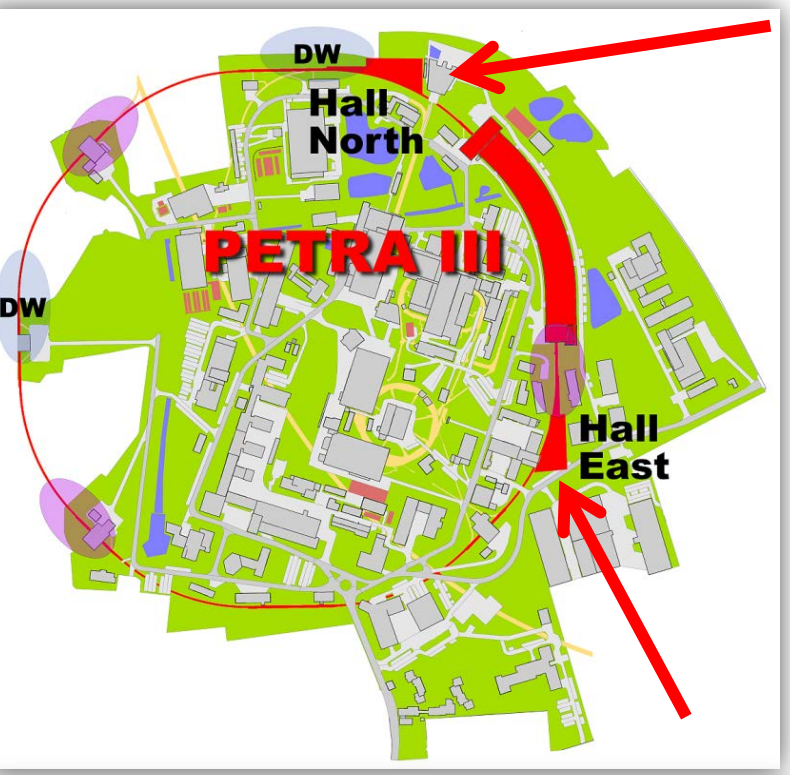
First Official Users (Helmholtz Centre for Heavy Ion Research, Darmstadt)

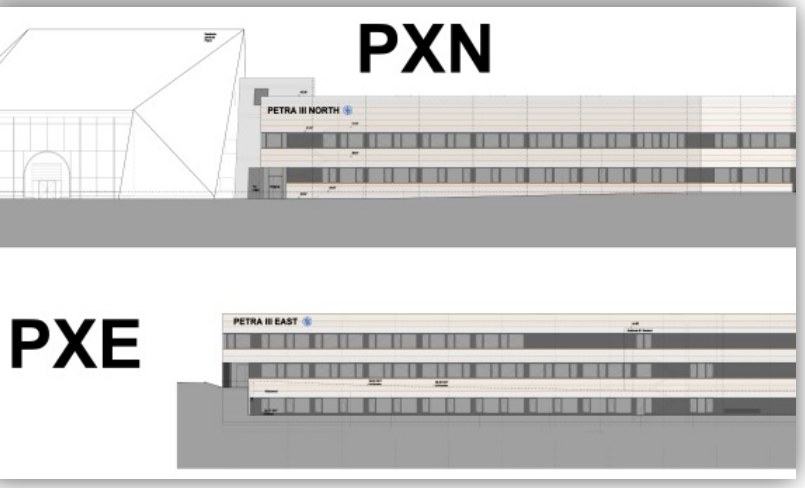
Beamlines: PETRA III

- P01 High Resolution Dynamics Beamline
- P02 Hard X-Ray Diffraction Beamline
- P03 MINAXS
- P04 XUV Beamline
- P05 Imaging Beamline
- P06 Hard X-Ray Micro Probe
- P07 High Energy Materials Science
- P08 High Res Diffraction
- P09 Resonant Scattering and Diffraction
- P10 Coherence Applications
- P11 Bio-Imaging and Diffraction
- P12 BioSAXS
- P13 Macromolecular Crystallography I
- P14 Macromolecular Crystallography II



UPGRADE: PETRA III extension

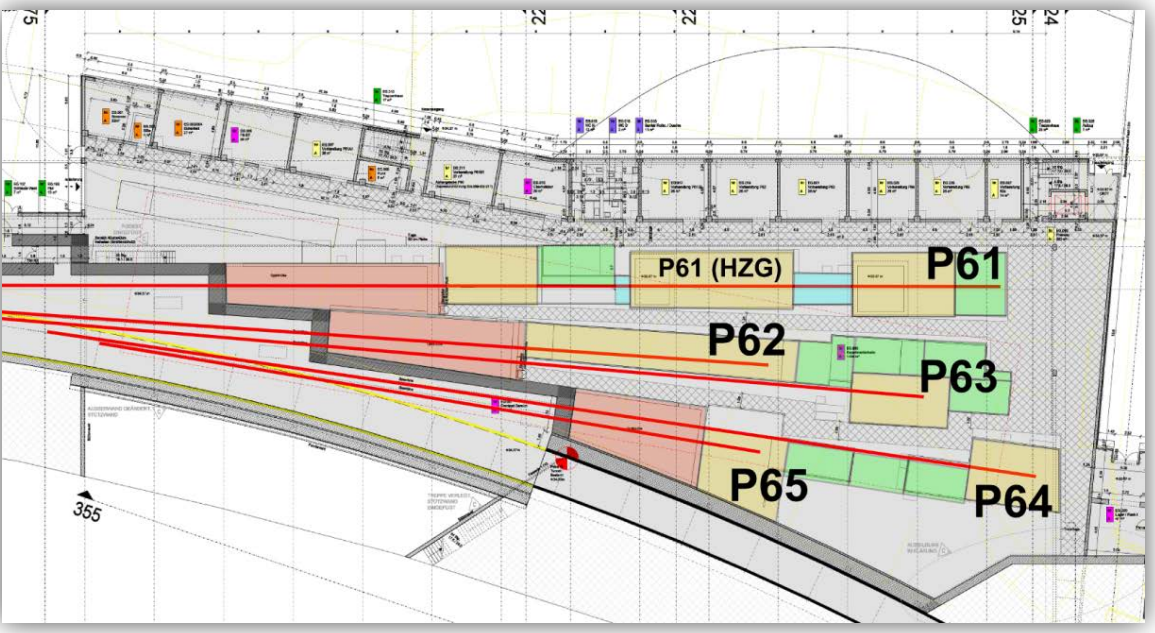




- After closure of DORIS III (36 beamlines) additional capacity is urgently needed
- Extension of PETRA III in progress
  - two new experimental halls (North and East)
  - construction starts January, 2014
  - due to machine shut down and re-commissioning no regular PETRA III user operation in 2014

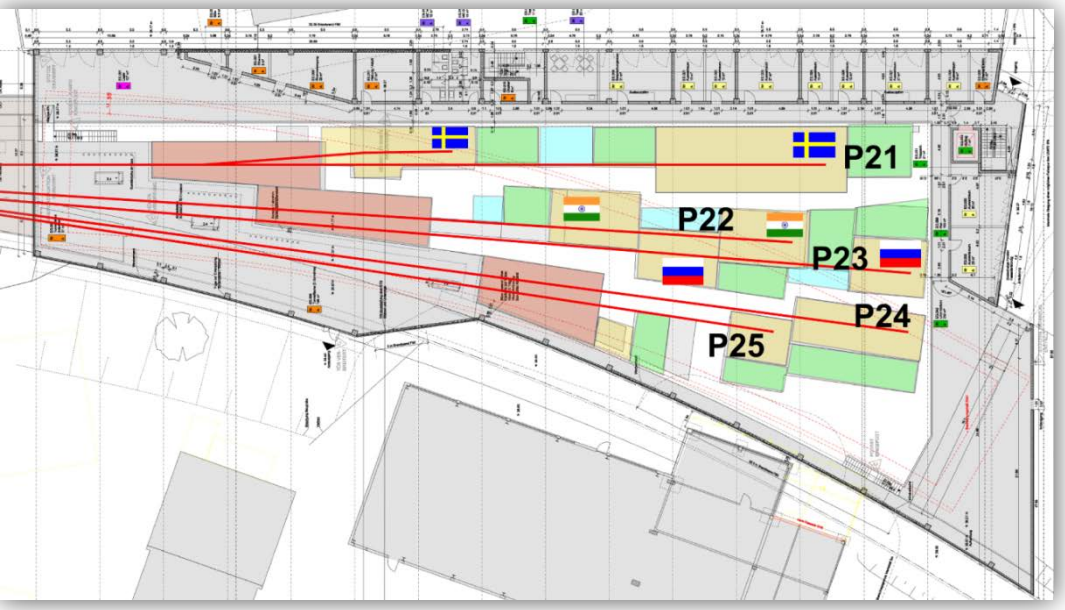
PETRA III Extension – Hall North Beamlines

- P61.1 - High-Energy Materials Science Beamline (HZG)
- P61.2 - High Pressure Extreme Conditions in a Large Volume Press (DESY) (2016)
- P62 - Small Angle X-ray Scattering Beamline (2016)
- *P63 - X-ray Micro-Fluorescence Spectroscopy Beamline (tentative – no funding)*
- **P64 - Time-Resolved- & Bio- X-ray Absorption Spectroscopy Beamline (Summer 2015)**
- **P65 - X-ray Absorption Spectroscopy Beamline (Summer 2015)**



PETRA III Extension – Hall East Beamlines

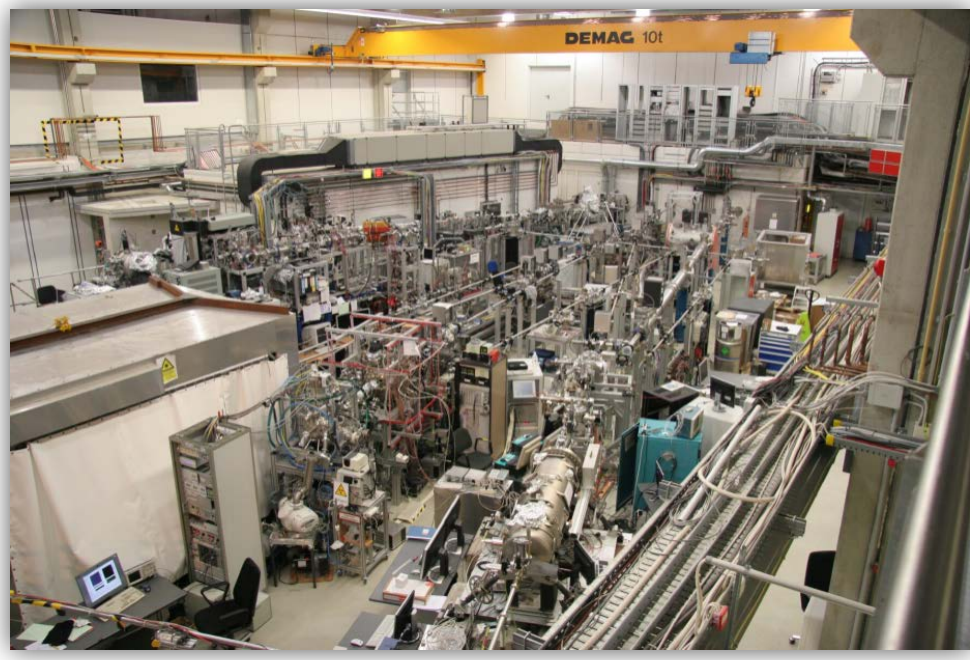
- P21.1 – **Swedish** High Energy Side Station (Spring 2016)
- P21.2 – **Swedish** High-Energy Materials Science Beamline (Fall 2015)
- P22 - **Indian/German** Nano-Spectroscopy Beamline
- P23 - **Russian/German** Nano-Diffraction Beamline (Fall 2015)
- P24 - Chemical Crystallography Beamline (Fall 2015)
- *P25 - Education, Training, Testing (not funded yet)*



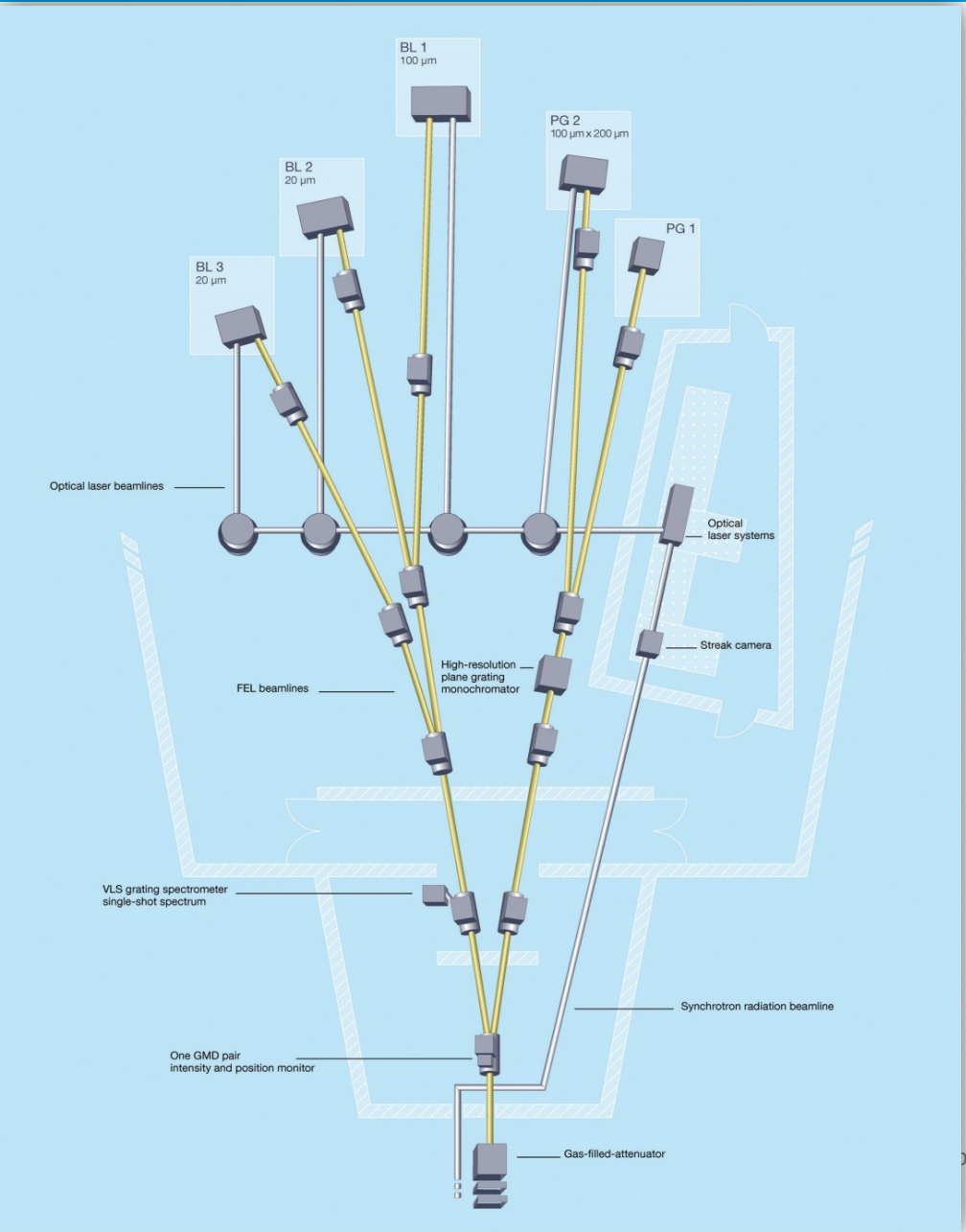
→ 3 beamlines built within international cooperations → special access contingents

FLASH- Free-Electron LASer in Hamburg

- User access since 2005
- first Free-Electron Laser with a superconducting linear accelerator
- presently the only FEL user facility in the ultraviolet and soft X-ray regime

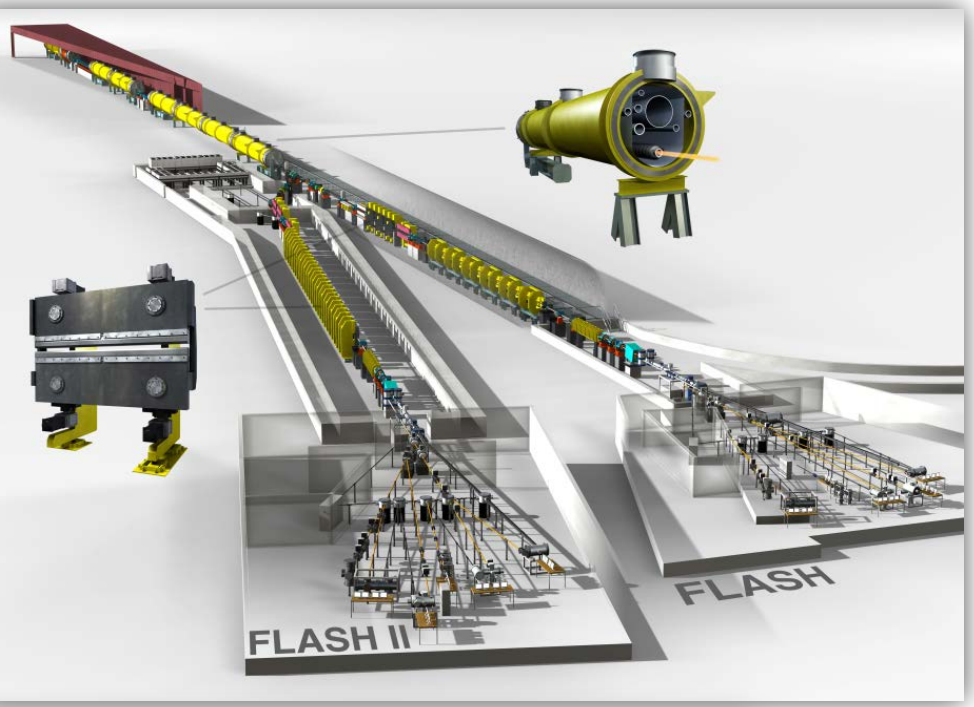


FLASH - Beamlines



- 5 beamlines operational (two experiments in parallel), PG 1 with permanent end station
- optical laser system is routinely provided for pump-probe experiments at all beamlines
- At present: Shut down until Oct 2013 for construction of FLASH II extension

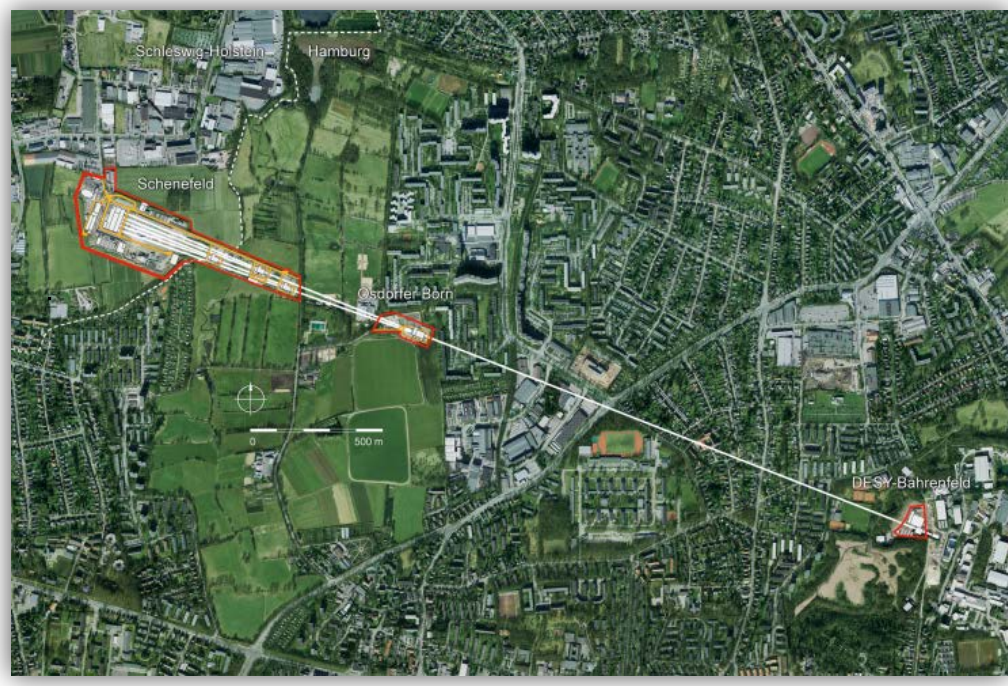
FLASH II - extension



- FLASH II tunnel construction started in 2011, tunnel and hall are being furnished at the moment
- new experimental hall for approximately six new photon beamlines & experimental stations
- double the user capacity of FLASH
- FLASH and FLASH II can be operated in parallel, with a largely independent adjustment of the wavelengths
- user experiments are expected to start in 2014

European X-Ray Free-Electron Laser XFEL

- 3.4 km long facility from DESY campus to Schenefeld
- DESY is largest shareholder
- DESY will also operate the accelerator
- nanometre-scale structures, fast processes, and extreme states
- 3D images of viruses and proteins, filming chemical reactions
- User access from 2015 on



Research Platforms: CFEL

> Center for Free-Electron Laser Science

- joint enterprise from DESY, the Max Planck Society (MPG), and the University of Hamburg.
- dedicated to the investigation of structural changes of atoms, molecules, condensed, biological, or warm dense matter

DESY is represented by

- 2 Experimental Research Divisions

- for *Coherent Imaging* of Henry Chapman including independent research group “Controlled Molecule Imaging” headed by Jochen Küpper

- for *Ultrafast Optics and X-rays* of Franz X. Kärtner

- CFEL *Theory Division* of Robin Santra

Research Platforms: DESY NanoLab

> DESY Nanolaboratory

- The DESY NanoLab is planned as a new on-site user facility
- construction autumn 2013-2015
- providing lab facilities for surface preparation and nanoparticle growth
- advanced nano-characterization & nano-structuring
- access will be provided in combination with approved beamtimes at PETRA III and FLASH

Figure by courtesy of REINER BECKER ARCHITEKTEN

Research Platforms: CSSB

> Centre for Structural Systems Biology

- new interdisciplinary centre on the DESY campus dedicated to infection research
- alliance of 9 universities and non-university research institutions
- office and lab space for about 150 scientific and technical staff from 2016 on
- DESY will provide direct and fast access to experimental facilities at PETRA III

CSSB
Centre for Structural
Systems Biology

Outstations: University Hamburg

> University of Hamburg

- **Institute for Experimental Physics**
- **Institute of Laser Physics**
- **Center for Optical Quantum Technologies**
- II. Institut für Theoretische Physik

- **PIER**- Partnership for Innovation, Education and Research
  founded in 2011: strong coordination of both institutions' research and training activities (i.e. graduate school), also promoting transfer of science and technology throughout the Hamburg region

PIER

Eine Partnerschaft der Universität Hamburg und DESY

Outstations: EMBL & HZG

Close cooperation at beamlines

> EMBL European Molecular Biology Lab Unit Hamburg

- Operating beamlines P11-13
- Separate Proposal + Review System
- run their own User Office

> Helmholtz-Centre Geesthacht

- German Engineering Materials Science Centre
- Beamlines P05 & P07
- Proposal System & User Administration via DESY System DOOR
- Chair one of the DESY Photon Science Proposal Review Panel

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

USER OFFICE – tasks & personnel

Head of Office: Daniela Unger (~0.8 FTE) (since Dec 2012)

- Communication
  - between users – beamline staff - IT (user portal DOOR)
  - On-site DESY departments
  - DESY Photon Science User Commitee
  - Other related organizations (on-site institutes, BiostructX, Komitee für Forschung mit Synchrotronstrahlung …..)
- Conceptional works, contribute to:
  - development of new proposal & report procedure (DOOR)
  - development of new publication database interface
  - development of legal user agreement, user guidelines & broschures …..
- Webpage
  - Users‘ Area (concept, keeping updated)
  - All user relevant aspects of Webpage

USER OFFICE– tasks & personnel

- Coordination Proposal Review Process & Meetings
- Editorial Work
  - User Experimental Reports
  - DESY Photon Science Annual Report
- Compilation of Numbers & Statistics (users, publications etc.)
- Preparation of Users‘ Meeting
- Travel Cost Reimbursement Control
- Request Tracker
- Publication appointee
- ….. miscellanous

USER OFFICE– tasks & personnel

Secretary: Maja Stolper (0.5 FTE)

- Handling of requests concerning
  - Registration of users
  - Changes of personal data entries
  - Travel reimbursement
  - Safety training & activation of certificates
  - Access Cards to Facilities
  - General user support
  - Visa support
  - ….

Support by DESY administration

- International Office (3 FTE)
  - invitation letters, applications for residence permits, visa extensions etc.
  - assistance with DESY requirements and procedures
  - medical and liability insurance for DESY guests
  - schools and daycare in Hamburg, kindergarten at DESY
  - general information on daily life in Hamburg
- Hostel
  - supplies rooms during experimental stays, conferences
  - 2 FTE plus external service personnel
- Housing (1 FTE)
  - assists in finding long-term housing (>4 weeks)
- IT, PR, Library, Conference Organisation, TT

COMMERCIAL USERS: Services by DESY

- Technology Transfer: Industrial Service Group
  - acts as contact and advise interested Commercial Users (in cooperation with DESY Photon Science)
  - Administration of commercial access
  - Customer Acquisition

    - Guided tours for interested companies
    - Website, Brochures
    - Exhibitions (Exhibitor and Guest)

- Rapid Access (2-8 weeks)
- To-be-published or confidential measurements
- standardized contracts and framework cooperation

By courtesy of Ilka Mahns/TT

COMMERCIAL USERS: access types

> Feasibility Studies:

- Check, if intended experiment at DESY is appropriate for research question
- Measurement time (incl. scientific support): 4 hours
- Free of charge

> Short-Term Access:

- Measurement time: minimum 4 hours
- Costs range from 550 € (published) to 786 € (confidential) per hour
- extra costs if complete measurement is done by DESY personnel

> Long-Term Cooperation:

- cooperation agreement between the company and DESY with an annual flat rate
- fast & flexible access to measurement times incl. support by Industrial Service Group
- conditions vary with duration of the cooperation & requests of the company

By courtesy of Ilka Mahns/TT

COMMERCIAL USERS: Access to DESY Photon Facilities

> Participation in SCIENCE LINK (2012-2014)

- network of the EU-Baltic Sea States
  Max IV Laboratory, Lund Sweden, DESY Hamburg, Helmholtz-Zentrum Berlin, Helmholtz-Zentrum Geesthacht offer free experiment time and consultation to new customers
- 9 applications during the first call, 21 during the second and 36 applications during the third call

> Commercial Access 2009-2012

	2009	2010	2011	2012
Companies	10	13	9	14
Measurement time [h] (DORIS III and PETRA III)	1.453	1.070	861	899

By courtesy of Ilka Mahns/TT

DESY Photon Science User Commitee (DPS-UC)

- elected by the users for a term of 3 years during the DESY Photon Science Users' Meeting
- at least 5 external members
- direct link Users - DESY Photon Science Management
- DPS-UC is kept informed on operation schedules and developments at DESY Photon Science
- gives recommendations for the scientific program of the users' meeting
- takes note of the users' needs and concerns regarding on-site work during experiments, operating procedures, general user support etc.
- complaints are confidential unless otherwise agreed with user
- Chair reports during Users' Meeting

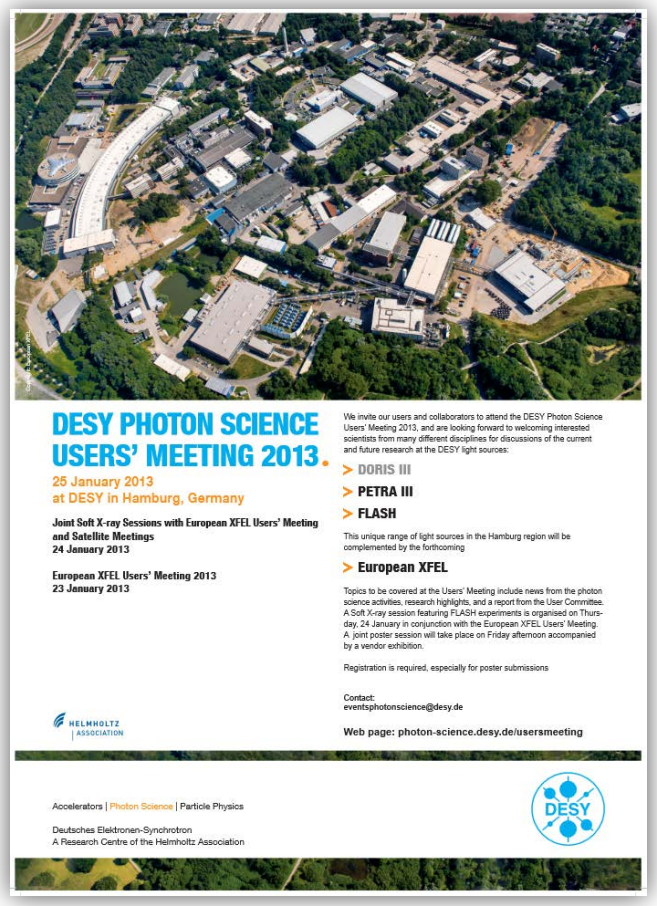
DPS-UC Members (from left to right):

Markus Perbandt
Christian Schroer
Peter Müller-Buschbaum (Chair)
Thomas Möller

Joachim Wollschläger

USER COMMUNITY: DESY Photon Science Users‘ Meeting

- Annual meeting of all interested Users
  - **fixed date**: last Friday in January
  - No conference fee
- Since 2013 two-days meeting together with European XFEL
- ~ 800 registrations in 2013



DESY PHOTON SCIENCE USERS' MEETING 2013.

25 January 2013
at DESY in Hamburg, Germany

Joint Soft X-ray Sessions with European XFEL Users' Meeting and Satellite Meetings
24 January 2013

European XFEL Users' Meeting 2013
23 January 2013

We invite our users and collaborators to attend the DESY Photon Science Users' Meeting 2013, and are looking forward to welcoming interested scientists from many different disciplines for discussions of the current and future research at the DESY light sources:

- DORIS III
- PETRA III
- FLASH

This unique range of light sources in the Hamburg region will be complemented by the forthcoming

- European XFEL

Topics to be covered at the Users' Meeting include news from the photon science activities, research highlights, and a report from the User Committee. A Soft X-ray session featuring FLASH experiments is organised on Thursday, 24 January in conjunction with the European XFEL Users' Meeting. A joint poster session will take place on Friday afternoon accompanied by a vendor exhibition.

Registration is required, especially for poster submissions

Contact:
eventsphotonscience@desy.de

Web page: photon-science.desy.de/usersmeeting

HELMHOLTZ ASSOCIATION

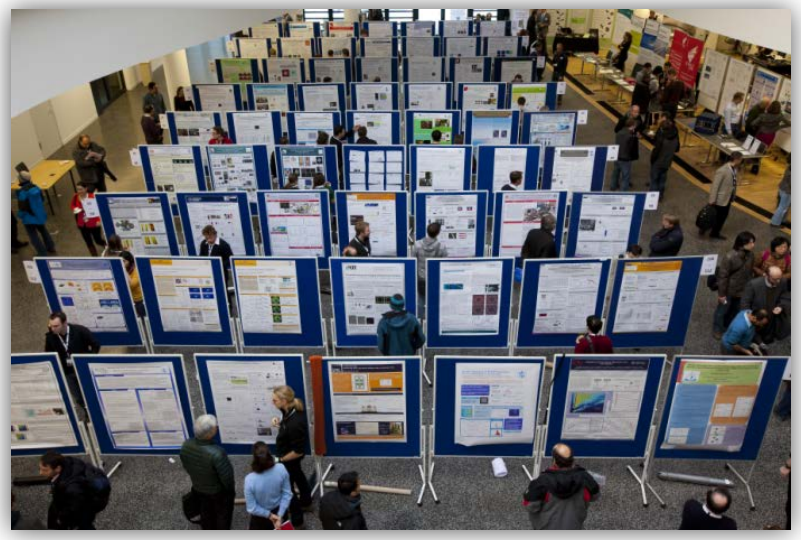
Accelerators | Photon Science | Particle Physics

Deutsches Elektronen-Synchrotron
A Research Centre of the Helmholtz Association

DESY

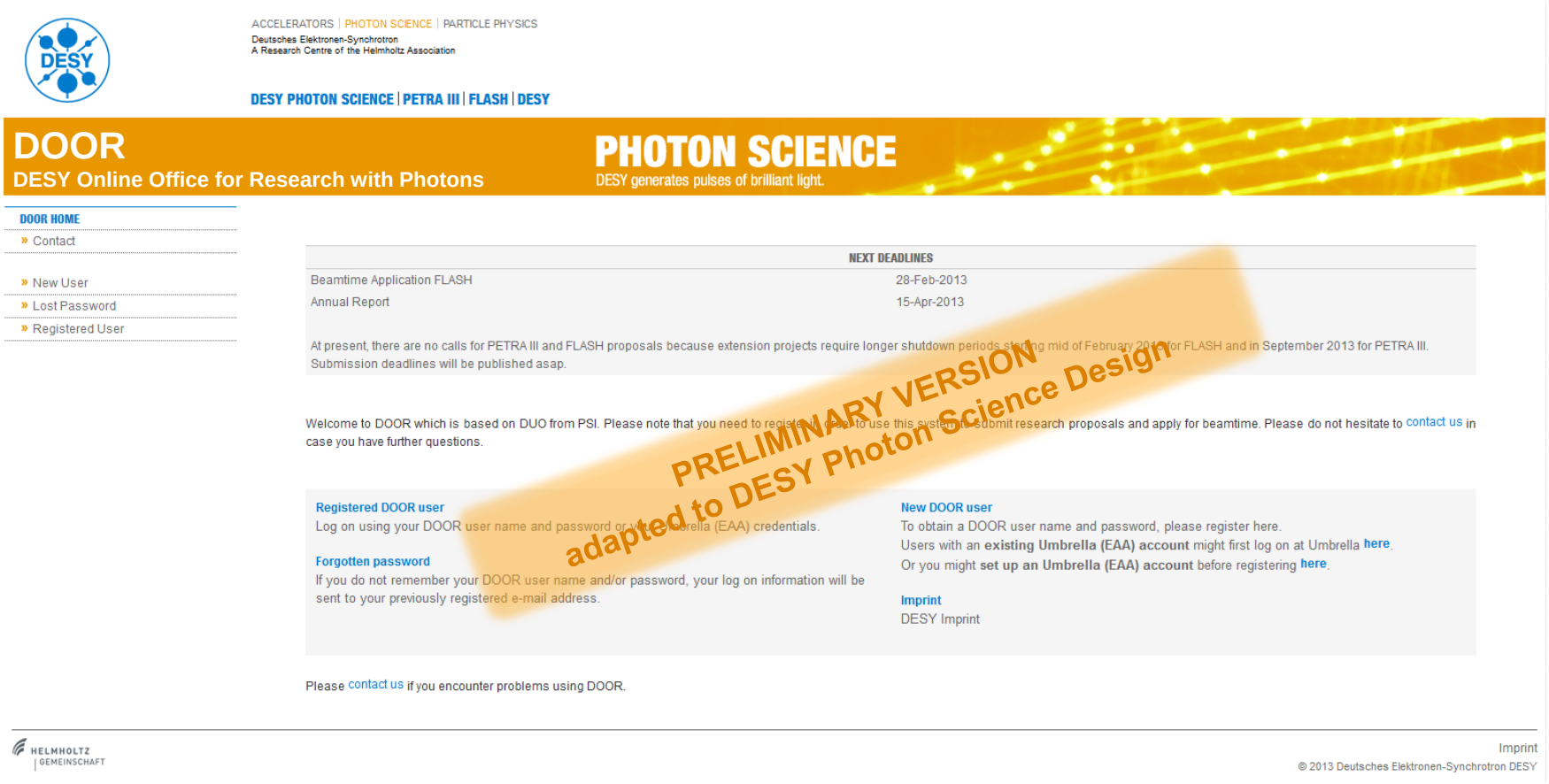
USER COMMUNITY : DESY Photon Science Users‘ Meeting

- Poster Session and Scientific talks
- Industry & Vendor Session
- Satellite Workshops on instrumentation and development

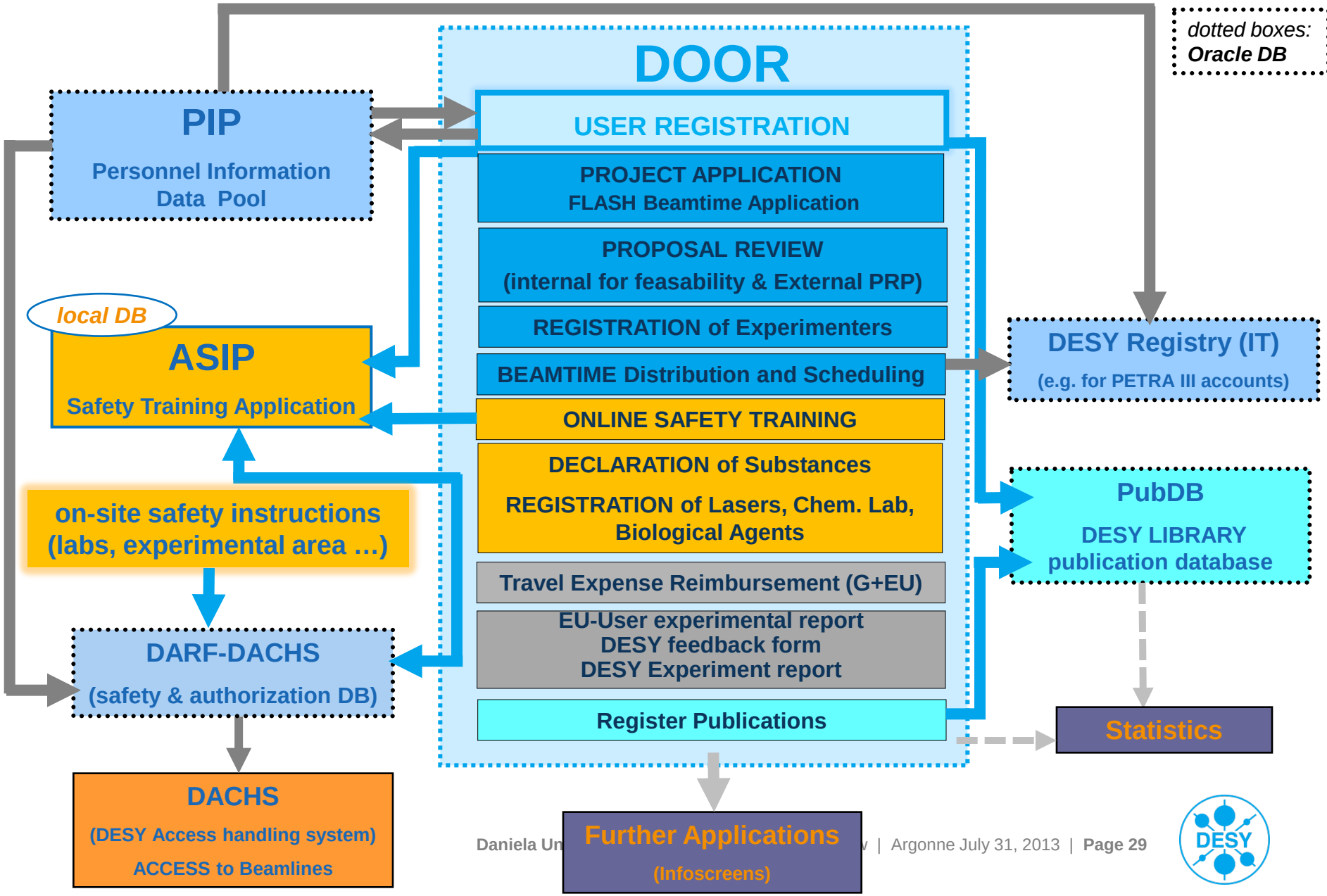


User Access to Photon Science Facilities

- Access to facilities is administrated via **DOOR** (**D**ESY **O**nline **O**ffice for **R**esearch with Photons) (based on DUO by PSI)
- **DOOR** is currently being re-structured and new version will be launched after PETRA III shutdown



DOOR – DESY Online Office for Research with Photons



DOOR Proposal submission: General Part

PROPOSAL SUBMISSION
GENERAL PART

Step 1: General part | Step 2: Beamline specification | Step 3: Detailed project description | Step 4: Submit proposal

TITLE (*)

Example Three-Way Meeting

LEADER/PRINCIPAL INVESTIGATOR

Project Leader (*)	Dr. Wolfgang Drube	[Select] [Remove]
Principal Investigator (*)	Dr. Daniela Unger	[Select] [Remove]

CO-PROPOSERS

Co-Proposer		[Select] [Remove]
Co-Proposer		[Select] [Remove]
Co-Proposer		[Select] [Remove]
Co-Proposer		[Select] [Remove]
Co-Proposer		[Select] [Remove]

EXPERIMENT SPECIFICATIONS

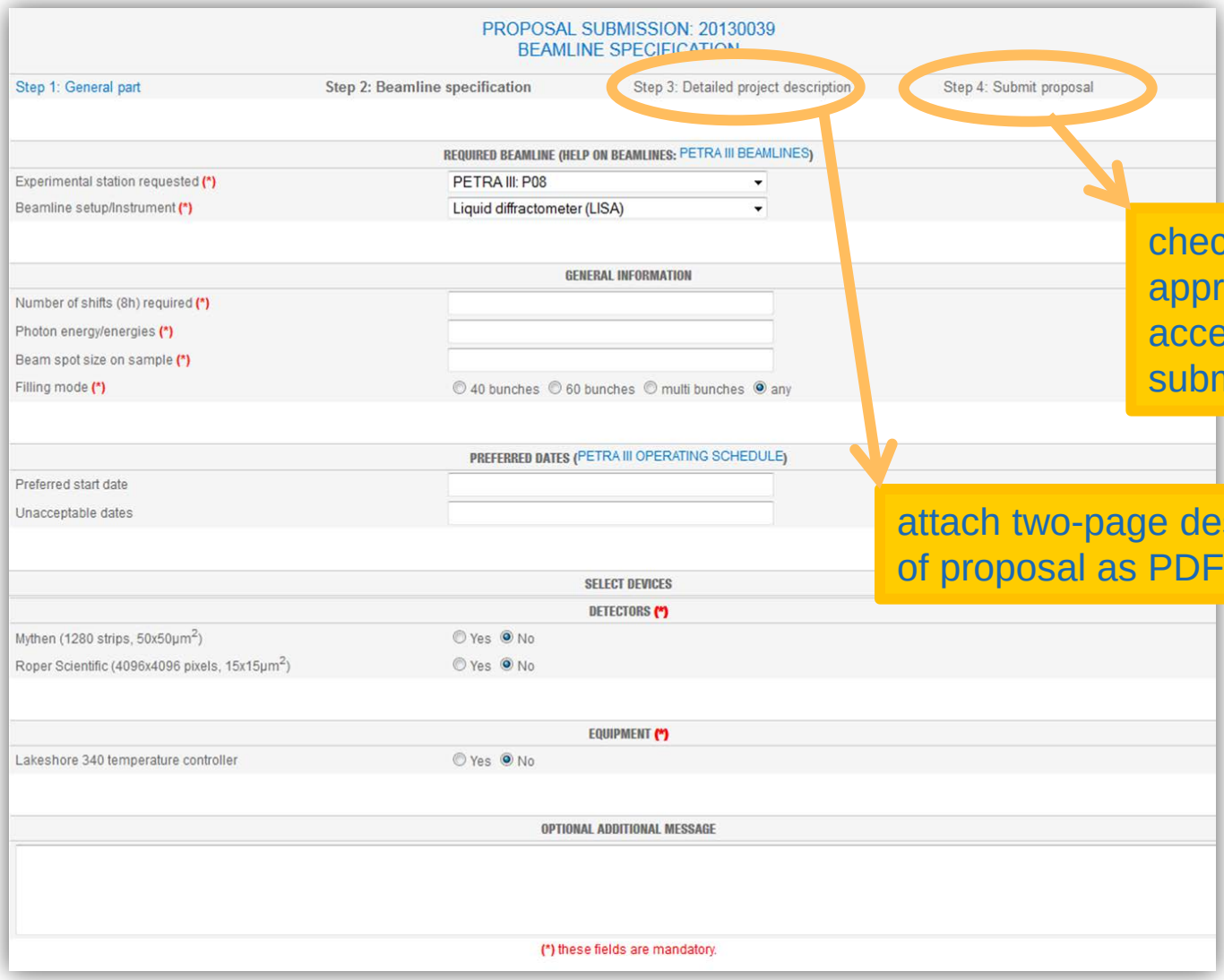
Experiment Type (*)	Short-term (valid 6 months)
Review Committee (*)	X-ray Spectroscopy
Primary Research Field (*)	Key technologies (including information and communication technologies)
Secondary Research Field	Transport and space
Research Category (*)	Industrially relevant
Proposals Type	General user

BRIEF DESCRIPTION OF THE PROPOSED EXPERIMENT (MAX 500 CHARACTERS) (*)

500 characters left

(*) these fields are mandatory.

DOOR Proposal submission: Beamline Specification



PROPOSAL SUBMISSION: 20130039
BEAMLINE SPECIFICATION

Step 1: General part | **Step 2: Beamline specification** | Step 3: Detailed project description | Step 4: Submit proposal

REQUIRED BEAMLINE (HELP ON BEAMLINES: PETRA III BEAMLINES)

Experimental station requested (*): PETRA III: P08
Beamline setup/Instrument (*): Liquid diffractometer (LISA)

GENERAL INFORMATION

Number of shifts (8h) required (*)
Photon energy/energies (*)
Beam spot size on sample (*)
Filling mode (*): 40 bunches | 60 bunches | multi bunches | any

PREFERRED DATES (PETRA III OPERATING SCHEDULE)

Preferred start date
Unacceptable dates

SELECT DEVICES

DETECTORS (*)

Mythen (1280 strips, 50x50µm^2): Yes | No
Roper Scientific (4096x4096 pixels, 15x15µm^2): Yes | No

EQUIPMENT (*)

Lakeshore 340 temperature controller: Yes | No

OPTIONAL ADDITIONAL MESSAGE

(*) these fields are mandatory.

check
approve
accept User Agreement
submit

attach two-page description
of proposal as PDF

BEAMTIME REQUEST: proposals

PETRA III

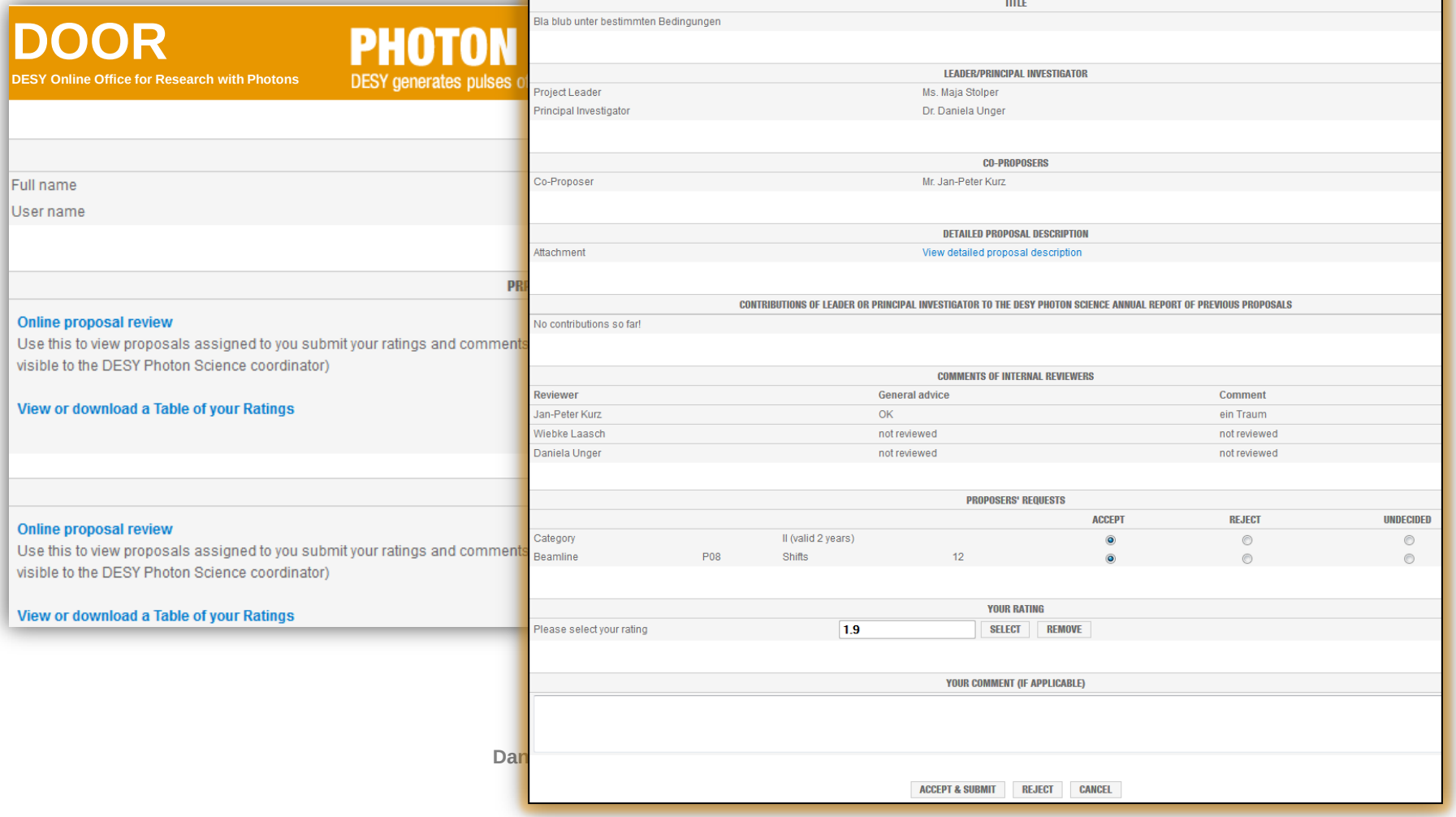
- Proposals: 2 calls per year (deadlines: 1 March & 1 September)
- Short term proposals
  - one-step proposal system, no extra beamtime application
  - validity ½ year
  - only one beamline can be selected
- Long term proposals
  - proposal submission as for short term
  - validity 3 years
  - in total 5 beamtime applications are possible
  - beamtime application along with regular proposal calls, i.e. 2 x per year

FLASH

- Irregular call periods, no beamline specification in DOOR, extra beamtime application always neccesary due to complexity of experiments

PROPOSAL REVIEW : Internal & External by PRP

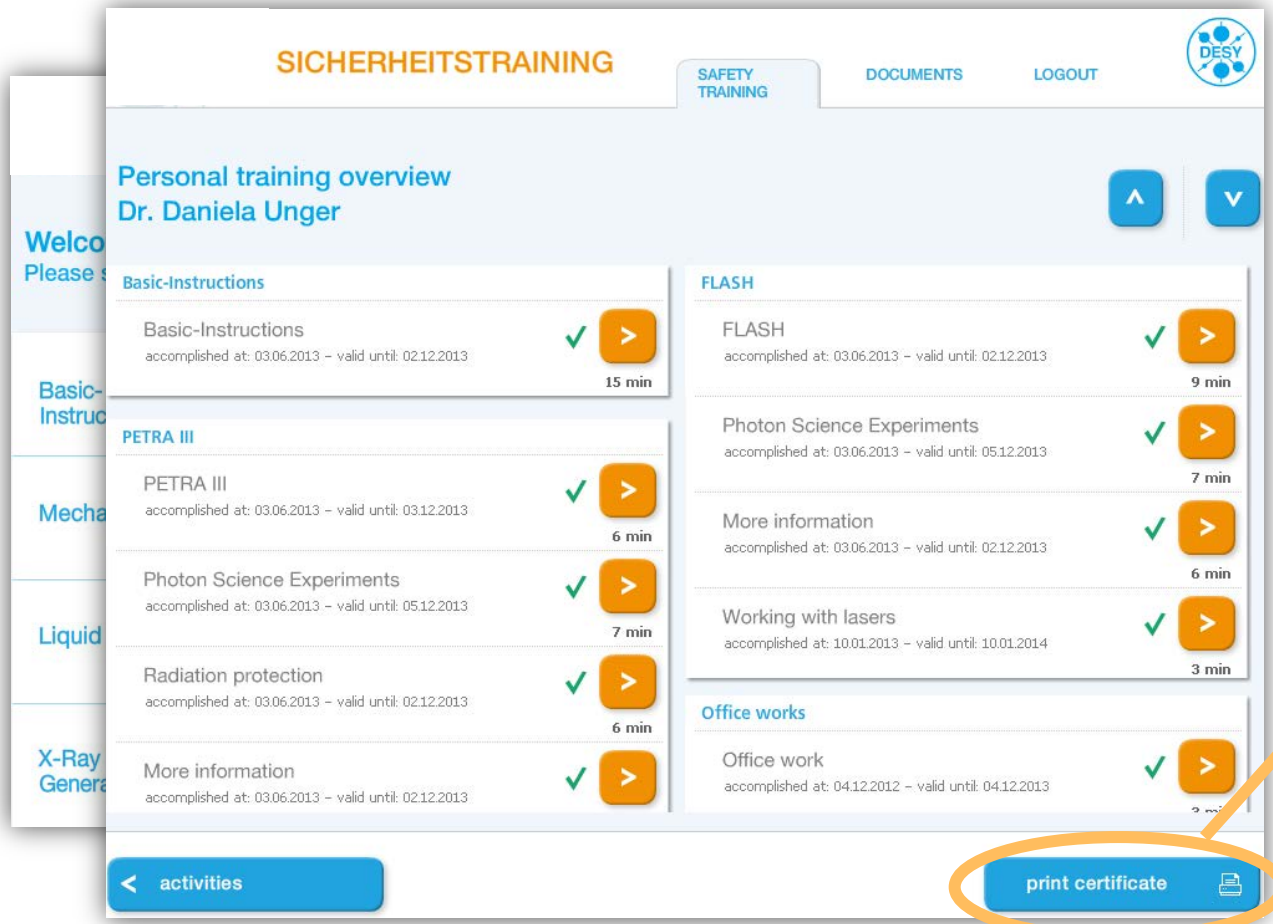
- Internal: Technical feasability
- External by PRP: Rating



SAFETY

> Online safety training ASIP

- Chose modules appropiate for experiment
- Validity 6-12 months



Send signed certificate to USER OFFICE for registration in DARF-DACHS

SAFETY

BEFORE COMING TO DESY

> Declaration of substances

> Registration of laboratory use, lasers, biological agents

→ checked by Beamline Scientist

→ if neccesary checked by Photon Science Safety Officers (Technical Infrastructure)

→ if further neccesary by DESY Safety Department

DURING STAY AT DESY BEFORE EXPERIMENT

> On-site instructions by beamline and lab team

→ fed into DACHS data base

USER EXPERIMENT FEEDBACK

should be delivered immediately after experiment,

but many users don’t

- **Success of experiment**
- **Machine reliability and Beam stability/quality**
- **Reason for beam loss**
- **Technical condition of experimental setup**
- **Scientific & technical support**
- **Administrative service**
- **Computing**
- **suggestions**

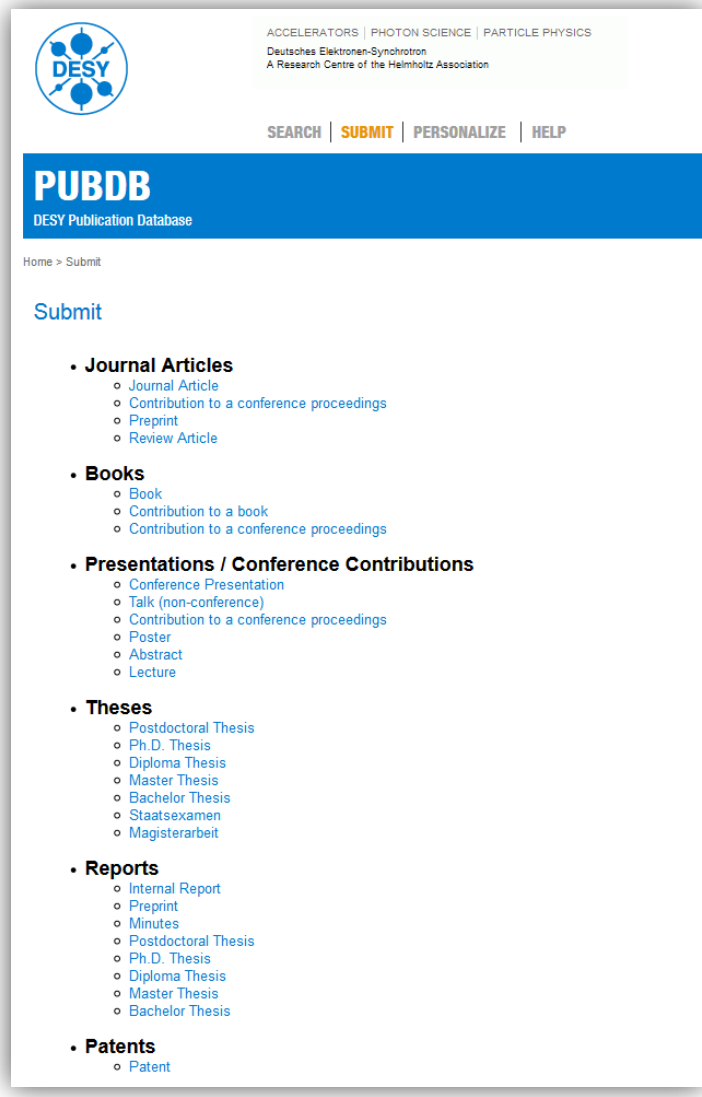
EXPERIMENTAL REPORT

- „Experimental Report“ will substitute „Contribution to Annual Report“ from 2014 on (after shutdown of PETRA III and relaunch of DOOR and the proposal system)
- due 3 months after Experiment
  - 1 page only
  - Should be absolutely mandatory!
- will not be published

PUBLICATIONS: how to collect

- Publications are collected via DESY Publication Database (PubDB)
- Users are directed to the PubDB via DOOR
- Submissions of users are cross-checked
  - by User Office (Publication Appointee)
  - Released by Library
- Problem: not all authors register their articles!

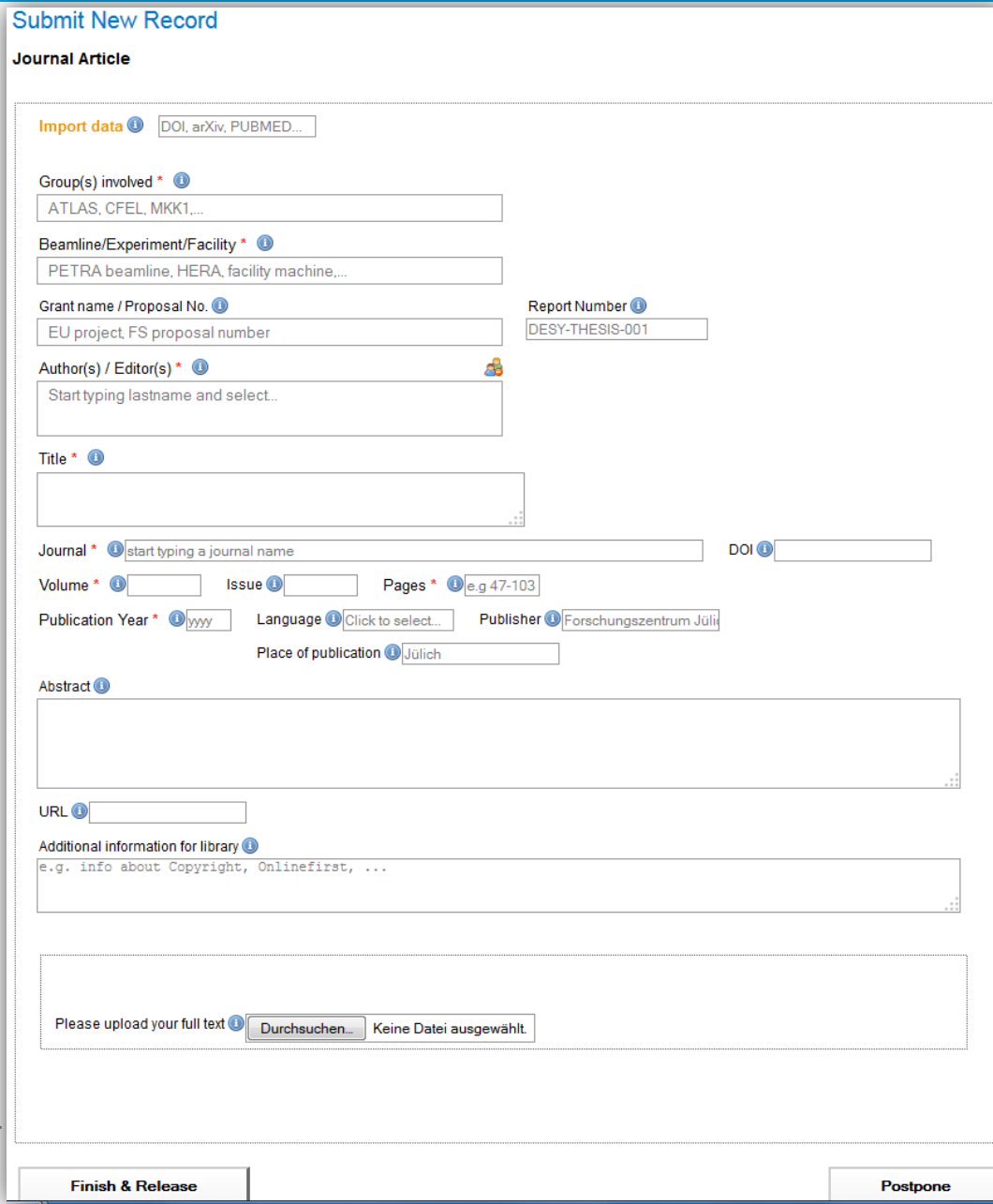
→ We try to „*complete*“ publication list by web search



PUBLICATIONS: how to collect

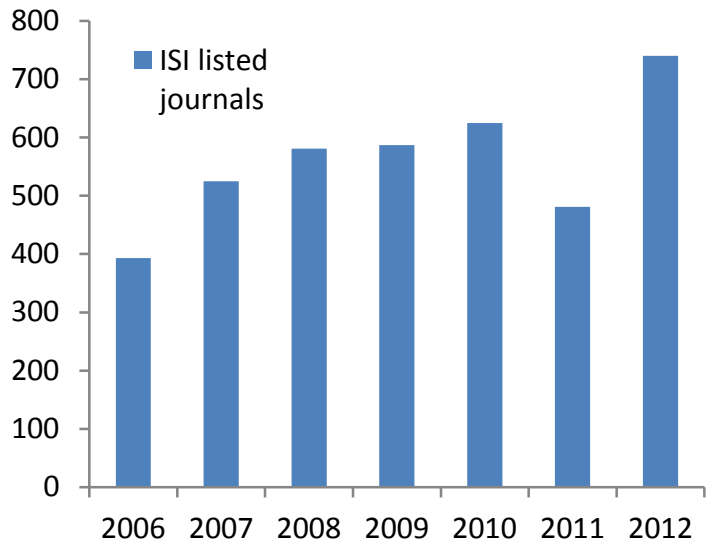
- Fast input with DOI, PUBMED, arXiv ID possible
- accomplished by info about groups, beamline, facility…
- Verification of identity of authors by comparison with DESY personnel database

→ important for exact publication statistics generated with PubDB

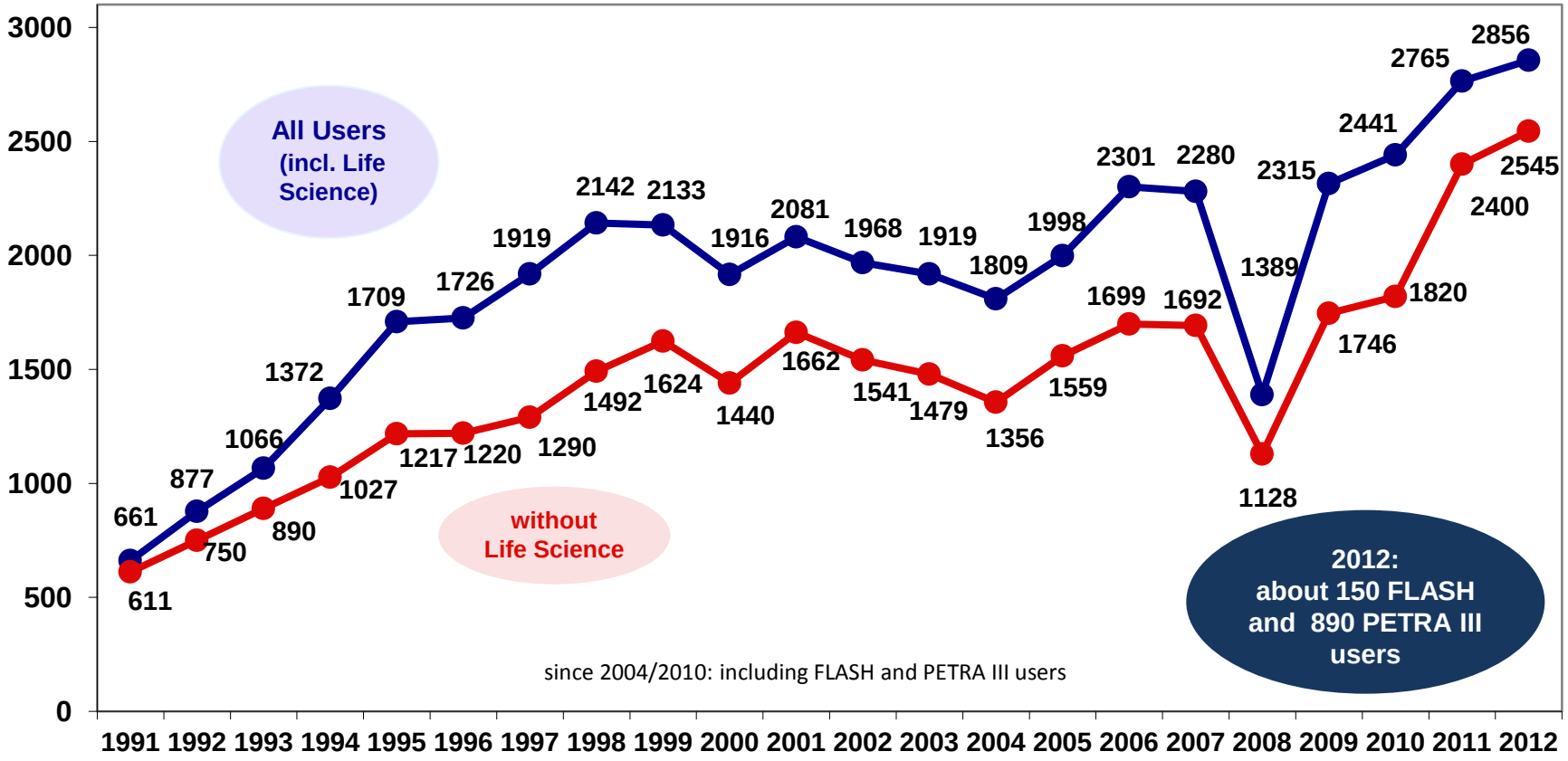


STATISTICS: ISI-Listed Publications

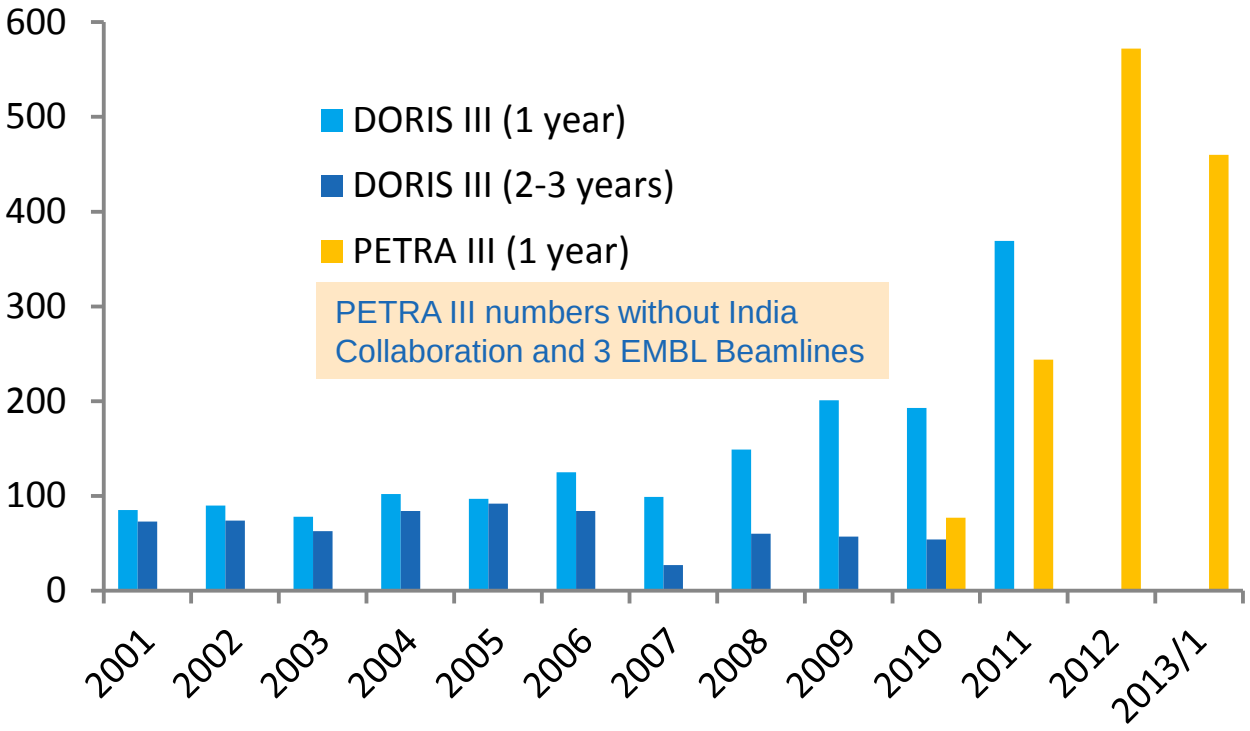
> Data retrieved from PubDB (operational since 2006)



STATISTICS – User numbers at DESY Photon Science



STATISTICS – Proposal numbers



> In 2013/1 high proposal numbers probably also due to upcoming shutdown

STATISTICS – Overbooking (Shifts)

year	DORIS III			PETRA III		
	Applied	Received		Applied	Received	
2010	16415	10048	1.6	1020	720	1.4
2011	14046	10241	1.4	3508	2303	1.5
2012	11032	8312	1.3	9664	4159	2.3

→ based on shifts applied for in beamtime applications (after approval of proposal)

period	FLASH		
	Applied	Received	
2010/11	948	324	2.9
2012/13	793	186	4.7

→ based on shifts applied for in proposal

ANNUAL BUDGET– Running Costs

> PETRA III (Million €)

Year	Machine	Experiments	TOTAL (incl. Overhead)
2010*	14.0	7.0	31.5
2011	14.7	10.8	38.25
2012**	15.0	11.9	40.35

* start official user operation
** fully operational

> FLASH (Million €)

Year	Machine	Experiments	TOTAL (incl. Overhead)
2010	13.8	2.8	24.9
2011	14.9	2.9	26.7
2012	15.1	3.9	28.5

EDUCATION & OUTREACH: Schools

- **practical training** in DESY's technical workshops and research groups (>14 years, after personal application)
- nationwide "**girls' day**": practical day especially for girls to promote their interest in natural and technical sciences
- "**physik.begreifen**" "grasp physics": pupils laboratory
  - vacuum (ca. 4th-8th grade / 9th-10th grade)
  - radioactivity
  - quantum physics (11th-13th grade)
  - particle physics (9th-10th grade)
  - e-lab (electron physics) (11th-13th grade)
  - cosmic rays master classes (at school or at DESY, >9th grade)
  - cosmic rays international Master Classes (2 weeks, 10th-13th grade)




EDUCATION & OUTREACH: general public

- **DESY guided tour** around the DESY site including a lecture
- annual "**Open Day**" "**Night of Science**" (>10.000 visitors in one day)
- monthly **Science Café DESY**: public afternoon lecture & discussion for pupils (>6th grade) and adults
- monthly **WISSENSWERTE**: public evening talks around Physics

Copyright: Daniel Drexelius

EDUCATION & OUTREACH: Students

- **International DESY Summer School** for undergraduates (physics, biology, chemistry, crystallography, material science, geology)
  - 100/30 students at DESY/Photon Science
  - lectures, experimental & research activities
  - 8 weeks

- **Fall School** - in cooperation with Uni Hamburg, 1 week
- **PIER Helmholtz Graduate School**

Acknowledgements

> Thanks for providing data & information and slides to

- Wiebke Laasch
- Ilka Mahns
- Wolfgang Drube
- Lucia Incoccia
- Jan-Peter Kurz

> Thank you for your attention

USER COMMUNITY: Workshops

- Mar. 2012: Inelastic X-ray Scattering Activities at PETRA III
- May. 2012: Workshop: German-Russian beamline at PETRA III Extension
- Jul. 2012: A2 achievements and future perspectives at PETRA III
- Sep. 2012: 2nd Workshop for Extreme Conditions Research in a Large Volume Press at PETRA III
- Oct. 2012: Science beyond 4 Mbar and using dynamic compression
- Jan. 2013 Users' Meeting

  -Nanoscience at large scale facilities: discussion of the DESY nanolab
  -3rd workshop on X-ray nano-imaging of biological and chemical systems at PETRA III
  -Status and Perspectives of Small-angle scattering at DESY
  -Extreme Conditions Research at DESY
  -The German Engineering Materials Science Centre (GEMS):
  Status and perspectives of the Helmholtz-Zentrum Geesthacht Outstation at DESY
  -High energy x-ray scattering at DESY
  -In Situ Rheology

- Mar 2013: Third German-Swedish workshop within the Röntgen-Ångström-Cluster on materials science
- Sep. 2013: Structural and in situ materials science at Beamline P02.1 @ PETRA III
- Oct. 2013: GISAXS 2013
- Oct. 2013: Workshop on High Pressure, Planetary, and Plasma Physics

USER EXPERIMENT FEEDBACK

> should be delivered immediately after experiment

1. which station or instrument was used for the experiment?
2. Overall success of your experiment?
3. Machine reliability during your experiments?
4. Beamtime lost during your experiment?

   Hours lost due to machine problems:

   Hours lost due to optics or controls problems:

   Hours lost due to end-station problems:

   Hours lost due to computing problems:

   Hours lost due to other problems:
5. How do you rate the photon beam quality (flux, stability, lifetime)?
6. Technical condition of the experimental setup?
7. Scientific and technical support provided by beamline staff?
8. Service provided by the DESY Photon Science user office?
9. Service provided by DESY (guest house, canteen, library, safety issues, etc)?
10. Local computing infrastructure and data handling?
11. Suggestions for improvements