



# DESY Photon Science Users' Meeting 2020 European XFEL Users' Meeting 2020

Jointly organized Users' Meeting of  
DESY Photon Science and European XFEL





**14th INTERNATIONAL CONFERENCE ON  
SYNCHROTRON RADIATION INSTRUMENTATION**

**SRI2021**

**30 August - 3 September 2021**  
CCH - Congress Center Hamburg





DESY Photon Science Users' Meeting 2020  
European XFEL Users' Meeting 2020  
in Hamburg, Germany  
DESY Auditorium (Bldg. 5)



Monday, 27 January: Satellite Workshops

<b>09:15 – 19:00</b>	Static Pressure Experiments at XFEL	<b>DESY   SemR</b> FLASH, Bldg. 28c
<b>13:30 – 18:30</b>	MID Workshop: First year of operation and future developments	<b>European XFEL  </b> XHQ E1.173
<b>13:30 – 18:30</b>	First experiments with a high-intensity short-pulse laser at HED/HIBEF	<b>European XFEL  </b> XTOB 1.01

Tuesday, 28 January: Satellite Workshops

<b>08:30 – 20:00</b>	Static Pressure Experiments at XFEL	<b>DESY   SemR</b> FLASH, Bldg. 28c
<b>09:30 – 13:00</b>	MID Workshop: First year of operation and future developments	<b>European XFEL  </b> XHQ E1.173
<b>09:30 – 12:00</b>	First experiments with a high-intensity short-pulse laser at HED/HIBEF	<b>European XFEL  </b> XTOB 1.01
<b>14:00 – 15:40</b>	User experience of data analysis at European XFEL	<b>DESY   CSSB</b> Lecture hall, Bldg. 15
<b>09:00 – 18:30</b>	Chemical Dynamics Opportunities at the FXE Instrument	<b>DESY   CFEL SemR</b> I-III, Bldg. 99
<b>13:00 - 19:00</b>	Current status and future completion at the HED instrument and the HIBEF contributions	<b>European XFEL  </b> XHQ E1.173

Wednesday, 29 January: European XFEL Users' meeting - Plenary Sessions

**8:30–10:00 Registration**

<b>10:15</b>	Welcome	R. Feidenhans'l	<i>EuXFEL</i>
<b>10:25</b>	Opening address from the Council Chair	M. Faury	<i>CEA Saclay</i>
	<b>European XFEL Update Session</b>		Chairperson: M. Faury (CEA)
<b>10:35</b>	General status of the project	R. Feidenhans'l	<i>EuXFEL</i>
<b>11:10</b>	Electron accelerator – status and further goals	W. Decking	<i>DESY Hamburg</i>
<b>11:45</b>	Requirements and ideas to reduce experiment data at EuXFEL	S. Aplin	<i>EuXFEL</i>
<b>12:20</b>	News from the European XFEL User Organization	A. Eschenlohr	<i>U Duisburg-Essen</i>

**12:40–14:00 Lunch break**

Science Session

Chairperson: O. Alekseeva (RAS)

<b>14:00</b>	Membrane protein MHz crystallography at the European XFEL	N. Zatsepin	<i>La Trobe</i>
<b>14:30</b>	Coulomb explosion imaging as structural probe of polyatomic molecules	R. Boll	<i>EuXFEL</i>
<b>15:00</b>	Insights into the donor-acceptor properties of base metal free dyads for photocatalysis	M. Bauer	<i>U Paderborn</i>
<b>15:30</b>	MHz X-ray Microscopy at Synchrotron and FEL Facilities	P. Vagovic	<i>DESY/EuXFEL</i>

**16:00-16:30 Coffee break**

Chairperson: M. Harmand (IMPMC)

<b>16:30</b>	Nucleation dynamics of skyrmion lattice from magnetic fluctuations phase	B. Pfau	<i>MBI Berlin</i>
<b>17:00</b>	Femto-second holographic X-ray imaging with FEL pulses of laser-induced cavitation bubbles	T. Salditt	<i>Uni. Göttingen</i>
<b>17:30</b>	Static high pressure experiments at European XFEL	S. McWilliams	<i>CSEC Edinburgh</i>
<b>18:00</b>	Elastic and inelastic X-ray scattering from isochorically heated carbon	D. Kraus	<i>HZDR</i>

**19:00 European XFEL Dinner Reception (in the DESY canteen, Bldg. 9)**

## Thursday, 30 January: DESY Photon Science Users' Meeting - FLASH

### 8:30–9:00 Registration

Chairperson: E. Plönjes (DESY)

09:00	Welcome	H. Franz	DESY Hamburg
09:05	FLASH - today and tomorrow - status report and future plans	M. Beye	DESY Hamburg
09:30	THz/XUV pump-probe experiments for studying local fields and dynamics at surfaces	J. Osterwalder	University of Zurich
10:00	Distorting atoms – The nonlinear driving of atom-specific transitions with intense XUV light	C. Ott	MPI-K Heidelberg

### 10:30 - 11:00 Coffee break

## Science Session: Soft X-ray FEL Science Highlights (jointly organised)

Chairperson: S. Molodtsov (EuXFEL)

11:00	X-ray Lasers Shed Light on the Mysteries of Water	A. Nilsson	U Stockholm
11:30	Imaging nanostructures in superfluid helium droplets	R. Tanyag	MBI Berlin
12:00	Evidence of Extreme Ultraviolet Superfluorescence in Xenon	L. Mercadier	EuXFEL
12:30	Transient magnetic scattering in thin Co/Pt multilayers upon femtosecond IR excitation	I. Pronin	University ITMO St. Petersburg
13:00	ESUO report	U. Pietsch (ESUO Chair)	Univ. Siegen

### 13.10 - 14.00 Lunch break

## Satellite workshops

13:00 - 18:25	10th workshop on X-ray Nano-Imaging of Biological and Chemical Systems at PETRA III	DESY   CFEL I-III, Bldg. 99
13:00–18:25	Coherent X-ray scattering and imaging	DESY   CFEL I-III, Bldg. 99 & SemR FLASH, Bldg. 28c
13:00–18:20	SAXS/WAXS/GISAXS User Workshop @ DESY	DESY   CSSB Lecture hall, Bldg. 15
14:00–19:00	High-pressure Science in the Large Volume Press at Beamline P61B	DESY   SemR 456, Bldg. 25f
14:00–18:40	Central infrastructure for DESY Photon Science Scientific computing - update and future directions	DESY   SemR. BAH1/BAH2, Bldg. 3
13:00–18:20	X-ray absorption spectroscopy at P64/65	DESY   SemR 4ab, Bldg. 1b
14:00–18:00	High Energy X-Ray Diffraction for Physics and Chemistry	DESY   CFEL SemR IV, Bldg. 99
14:00–18:00	Light-Matter Interaction: Recent Advances in Theory	DESY   CFEL SemR V, Bldg. 99
14:00–18:00	ECB Workshop (Extreme Conditions Beamline P02.2)	DESY   SemR 3, Bldg. 1b
14:00–18:30	Interfaces in electrochemistry, corrosion and solution based self assembly	DESY   SemR 109, Bldg. 25b
14:00–18:00	High Energy X-Rays for Swedish Materials Science	DESY   O1.030, Bldg. 48f
14:00–19:10	First meeting of the European XFEL Spanish user community	DESY   EMBL SemR, Bldg. 48e
14:00–18:00	Helmholtz-Zentrum Geesthacht GEMS Outstation: Materials Research and High Resolution Imaging	DESY   DESY Auditorium, Bldg. 5
14:00–18:00	Best of Science for new Therapies (on invitation)	DESY   SemR 1, Bldg. 1

19:00 DESY Reception for speakers and participants  
Supported by industry exhibition

(in the DESY canteen, Bldg. 9)



## Friday, January 31: DESY Photon Science Users' Meeting

### 8:30 – 9:00 Registration

Chairperson: G. Grübel (DESY)

09:00	Welcome and news from LEAPS	H. Dosch	DESY, Hamburg
09:10	Photon Science at DESY	E. Weckert	DESY, Hamburg
09:50	PETRA III and future outlook - PETRA IV	C. Schroer	DESY/Univ. Hamburg

### 10:20 - 10:50 Coffee break

Chairperson: H.-C. Wille (DESY)

10:50	Structural insights into the multifunctional L protein of bunyaviruses	M. Rosenthal	BNI Hamburg
11:20	Size Induced Structural Changes in Molybdenum Oxide Nanoparticles	T. L. Christiansen	Univ. Kopenhagen
11:50	Investigating Amphiphilic Monolayers with Grazing-Incidence Diffraction and X-ray Fluorescence	E. Schneck	TU Darmstadt
12:20	Direct imaging of orbitals in quantum materials using inelastic X-ray scattering	L. H. Tjeng	MPI Dresden
12:50	Report of the DESY Photon Science User Committee (DPS-UC) <b>Results DPS-UC Election 2020</b>	P. Müller-Buschbaum (DPS-UC Chair)	TU München
13:00	Report of the ‚Komitee Forschung mit SR‘ (KFS)	B. Murphy (KFS Chair)	University Kiel

### 13.10 - 14:00 Lunch break

14:00-17:00 POSTER SESSION (14-17h) and Vendor exhibition (10-18h)

Venue: "Kuppel Hamburg"

(dome on the Trabrennbahn Bahrenfeld, opposite to the campus - Luruper Chausse 30)

## DESY Photon Science User Committee

### Election 2020

Please vote **X** online until

Thursday 30 January, 14:00 h

**DOOR.desy.de**

## General Information

### Oral and poster sessions

The oral sessions will be held in the DESY auditorium (bldg. 5).

The poster session on Friday afternoon will take place in the dome 'Kuppel Hamburg'.

The 'Kuppel Hamburg' is located on the Trabrennbahn Hamburg, outside of the DESY campus near the side gate: Luruper Chaussee 30, 22761 Hamburg (see map).

### Vendor exhibition

The vendor exhibition will take place in the 'Kuppel Hamburg' on Friday, 31 January from 10 - 18h.

### Social events

#### The European XFEL reception

Wednesday, 29 January, at 19:00 in the DESY canteen (bldg. 9).

#### The DESY Photon Science reception

Thursday, 30 January, at 19:00 in the DESY canteen (bldg. 9).

### DESY WLAN

Name: UsersMeeting2020

WPA/WPA2-PSK: Ee7foi9koht4



### Organisers

S. Bertini (European XFEL), K. Baranašić (European XFEL), G. Heeßel (European XFEL), M. Kreuzeder (DESY), K. Kucza (DESY), W. Laasch (DESY), F. Lehmkuhler (DESY), S. Molodtsov (European XFEL), G. Quondam (European XFEL), A. Rothkirch (DESY), D. Unger (DESY)

## Local Information

### Cash machine/ATM

You will find a cash machine in the foyer of the DESY canteen (bldg. 9).

### Meals

#### Breakfast

If you stay at the DESY guest house you may have breakfast in the DESY cafeteria (opens at 07:00, bldg. 9) or CFEL Cafeteria (opens at 8:00, bldg. 99) at your own expenses.

#### Lunch

You may have lunch in the DESY canteen (bldg. 9) or CFEL Cafeteria (bldg. 99) at your own expenses.

### Shops etc.

Lidl (supermarket)

From the DESY main gate (Notkestrasse) turn right and follow the street (700 – 800m).

Denn's Biomarkt (supermarket)

From the DESY main gate walk straight down the street 'Zum Hünengrab' (700 – 800m). At the end of the street on the right side you will find the supermarket. You will find e.g. a bakery, drugstore and other shops as well as restaurants in the vicinity.

### Public transportation

*Bus (HVV):* Bus stops near the main entrance: 'Zum Hünengrab (DESY)' and near the side entrance: 'Luruper Chaussee (DESY)'. Further information: [www.hvv.de](http://www.hvv.de)

*Bike rental (StadtRAD Hamburg):* There are two city bike stations on the DESY campus where bikes can be returned. Further information: [stadtrad.hamburg.de](http://stadtrad.hamburg.de)

*On-demand shuttle service (ioki):* Stations are available in an area close to DESY and on the campus. Further information (a HVV ticket is needed in addition): [www.hvv.de/de/ioki](http://www.hvv.de/de/ioki).



**I Main sessions**  
**Abstracts of the talks**

## Membrane protein MHz crystallography at the European XFEL

Chris Gisriel<sup>1,2,3</sup>, Jesse Coe<sup>1,2</sup>, Romain Letrun<sup>4</sup>, Oleksandr M. Yefanov<sup>5</sup>, Cesar Luna-Chavez<sup>1,2</sup>, Natasha E. Stander<sup>1,2</sup>, Stella Lisova<sup>1,6</sup>, Valerio Mariani<sup>5</sup>, Manuela Kuhn<sup>5</sup>, Steve Aplin<sup>5</sup>, Thomas D. Grant<sup>7,8</sup>, Katerina Dörner<sup>4</sup>, Tokushi Sato<sup>4,5</sup>, Austin Echelmeier<sup>1,2</sup>, Jorvani Cruz Villarreal<sup>1,2</sup>, Mark S. Hunter<sup>9</sup>, Max O. Wiedorn<sup>5,10,11</sup>, Juraj Knoska<sup>5</sup>, Victoria Mazalova<sup>5</sup>, Shatabdi Roy-Chowdhury<sup>1,2</sup>, Jay-How Yang<sup>1,2</sup>, Alex Jones<sup>1,2</sup>, Richard Bean<sup>4</sup>, Johan Bielecki<sup>4</sup>, Yoonhee Kim<sup>4</sup>, Grant Mills<sup>4</sup>, Britta Weinhausen<sup>4</sup>, Jose D. Meza<sup>4</sup>, Nasser Al-Qudami<sup>4</sup>, Saša Bajt<sup>12</sup>, Gerrit Brehm<sup>1,2,13,14</sup>, Sabine Botha<sup>6</sup>, Djelloul Boukhelef<sup>4</sup>, Sandor Brockhauser<sup>4,15</sup>, Barry D. Bruce<sup>16,17,18</sup>, Matthew A. Coleman<sup>19</sup>, Cyril Danilevski<sup>4</sup>, Erin Discianno<sup>1</sup>, Zachary Dobson<sup>1,2</sup>, Hans Fangohr<sup>4,20</sup>, Jose M. Martin-Garcia<sup>1</sup>, Yaroslav Gevorkov<sup>8,21</sup>, Steffen Hauf<sup>4</sup>, Ahmad Hosseinizadeh<sup>21</sup>, Friederike Januschek<sup>4,22</sup>, Gihan K. Ketawala<sup>1,2</sup>, Christopher Kupitz<sup>9,21</sup>, Luis Maia<sup>4</sup>, Maurizio Manetti<sup>4</sup>, Marc Messerschmidt<sup>1,2,4</sup>, Thomas Michelat<sup>4</sup>, Jyotirmoy Mondal<sup>16</sup>, Abbas Ourmazd<sup>21</sup>, Gianpietro Previtali<sup>4</sup>, Iosifina Sarrou<sup>5</sup>, Silvan Schön<sup>5</sup>, Peter Schwander<sup>21</sup>, Megan L. Shelby<sup>19</sup>, Alessandro Silenzi<sup>4</sup>, Jolanta Sztuk-Dambietz<sup>4</sup>, Janusz Szuba<sup>4</sup>, Monica Turcato<sup>4</sup>, Thomas A. White<sup>5</sup>, Krzysztof Wrona<sup>4</sup>, Chen Xu<sup>4</sup>, Mohamed H. Abdellatif<sup>5</sup>, James D. Zook<sup>1,2</sup>, John C. H. Spence<sup>1,6</sup>, Henry N. Chapman<sup>5,10,11</sup>, Anton Barty<sup>5</sup>, Richard A. Kirian<sup>1,6</sup>, Matthias Frank<sup>19</sup>, Alexandra Ros<sup>1,2</sup>, Marius Schmidt<sup>21</sup>, Raimund Fromme<sup>1,2</sup>, Adrian P. Mancuso<sup>4,24</sup>, Petra Fromme<sup>1,2</sup> and Nadia A. Zatsepin<sup>1,6,24</sup>

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The presentation will focus on the first membrane protein megahertz serial femtosecond crystallography experiment at the SPB/SFX beamline of the European XFEL. We determined a high-resolution structure of the large membrane protein complex involved in photosynthesis, Photosystem I. The talk will cover challenges in megahertz SFX for membrane protein microcrystals, briefly covering batch microcrystallisation and sample delivery for MHz SFX, while focusing on data collection and analysis [1].

[1] Gisriel, C., Coe, J. et al. Nature Comm. 10, 5021 (2019) DOI: 10.1038/s41467-019-12955-3

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# Coulomb explosion imaging as structural probe of polyatomic molecules

Rebecca Boll

*European XFEL, SQS Scientific Instrument*

Recording images of individual molecules with ultrashort "exposure times" has been a long-standing dream in molecular physics, chemistry, and biology because this would allow one to follow the motion of atoms on their inherent timescale ( $10^{-15}$  s). While X-ray and electron diffraction have been successfully used to retrieve the structure of large biomolecules, both are very challenging to apply to small molecules in the gas phase. Moreover, these techniques are essentially blind to hydrogen atoms, which are key to many chemical reactions.

In one of the first user experiments at the Small Quantum Systems (SQS) instrument, we have used the very intense, femtosecond soft X-ray pulses from the European XFEL to record snapshot images of the complete structure of a molecule with eleven atoms, including all hydrogens, by Coulomb explosion imaging (CEI) using the reaction microscope (REMI) end station. Up to now, it was generally expected that, in order to image polyatomic molecules, it would be necessary to record essentially all charged fragments in coincidence – a requirement that is currently impossible to fulfil for more than a few atoms within a reasonable measurement time. However, here we demonstrate that, while it was possible to record up to six-fold ion coincidences in the experiment, even three-fold ion coincidences can be sufficient to image the full structure of a molecule. The X-ray intensity at SQS (up to  $10^{13}$  photons/ $\mu\text{m}^2$ ) is high enough to produce extreme charge states in heavy atoms (e.g. up to 42+ in xenon atoms), and to Coulomb-explode molecules into individual atoms very quickly, such that the initial molecular structure is well preserved in the recorded momenta of all ions.

The intriguingly clear momentum images allow us to identify each atom's position in the molecule unambiguously, and thus make it possible to trace the rearrangement of charge from the absorbing heavy atom to the other atoms in the molecule. Moreover, by combining our experimental results with state-of-the-art molecular dynamics calculations, we are able to follow in detail the charge-up dynamics of the molecule throughout the femtosecond X-ray pulse, thus gaining unprecedentedly detailed insights into the ultrafast charge rearrangement and fragmentation dynamics.

Given the femtosecond X-ray pulse duration, the presented results can, in the next step, readily be employed to monitor the temporal evolution of the molecular structure in a pump-probe experiment – thus bringing the long-standing dream of recording molecular movies of photo-chemical reactions very close to realisation.

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# Insights into the donor-acceptor properties of base metal free dyads for photocatalysis

Matthias Bauer

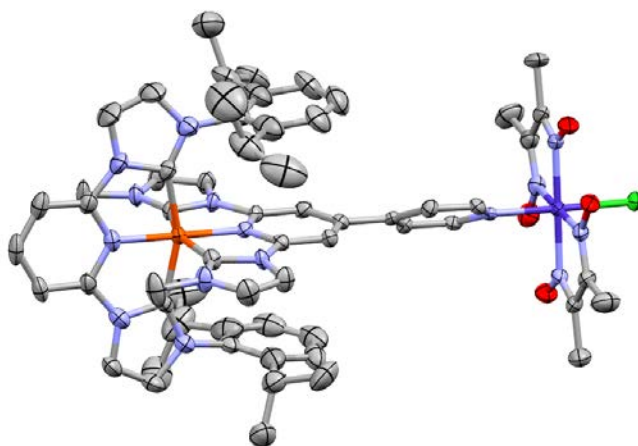
*University of Paderborn, Faculty of Science, Warburger Str. 100, 33098 Paderborn*

The conversion of sunlight into fuels or chemicals gains lots of attention by the so-called Sun-to-X approach. The reduction of protons to hydrogen using sunlight is one of the prototype reactions here. In particular with the renaissance of fuel cells as an alternative to batteries, sustainable hydrogen production becomes even more important.

While two-component proton reduction systems employ photosensitisers and catalysts in a diffusion driven process, molecular assemblies of both, so-called dyads could offer a vectorial electron transfer. This could reduce the lifetime limitations for the electron transfer in photocatalytic reactions.

Using base metals instead of noble metals increases the sustainable character of photocatalytic proton reduction. Both in photosensitizers and photocatalysts, metals like iron and cobalt can be used, but so far, no photocatalytically active dyads using only base metals exist. Achieving competitive activity of such noble-metal-free dyads requires major efforts in chemical design. Due to the very limited knowledge about the properties and functionality of base metal compounds in this context, fundamental insights into their working principle are mandatory.

X-ray emission and absorption spectroscopy (XES) provides unique details about the electronic and geometric structure of iron and cobalt photosensitisers and photocatalysts<sup>1</sup>. In particular for Fe-Co dyads as shown in Fig. 1, ultrafast cutting edge two-colour emission experiments<sup>2</sup> at the European XFEL and other X-ray free electron lasers are possible and of unique advantage to understand the electron transfer properties after photoexcitation. In these experiments, which will be presented in detail with this contribution, the emission lines of both metal sites in dyads are probed simultaneously, avoiding ambiguities in time zero and showing unprecedented new insights into the excited state behaviour of this new compound class. The obtained results indicate that a simple view on the electron transfer is not appropriate and needs to be exchanged by a detailed picture to achieve optimal photocatalytic activity.



**Figure 1.** X-ray structure of a bimetallic dyad using iron as photosensitiser and cobalt as catalyst.

## References

- [1] M. Bauer, M. Phys. Chem. Chem. Phys. 2014, 16, 13827.
- [2] A. Kalinko, W. Caliebe, R. Schoch, M. Bauer, J. Synchrotron Rad. 2020, 27, 31.

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# MHz X-ray Microscopy at Synchrotron and Free Electron Laser Facilities

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Modern emerging technologies, such as additive manufacturing, bio-printing, and new material production and processing, require novel metrology tools to probe fundamental high-speed dynamics happening in such systems. Such processes are stochastic in nature and conventional pump and probe stroboscopic approaches are not sufficient to provide accurate information about their complex nature. We present the application of the megahertz European X-ray Free-Electron Laser (EuXFEL) and Synchrotron sources to image the such fast stochastic processes and discuss future possibilities and applications of this method especially at new MHz rate

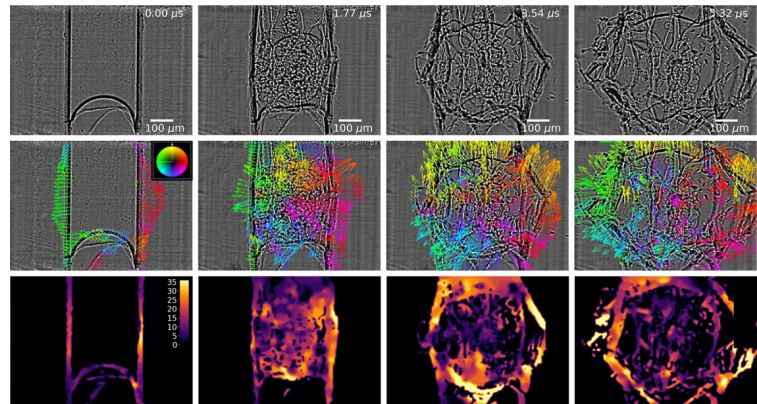


Figure 1: X-ray sequence of laser-induced dynamics in water filled glass capillary imaged at 1.13 MHz sampling rate (top) and processed velocity vectors (middle) and velocities (bottom).

XFEL photon sources. We present a first demonstration of the MHz X-ray microscopy method performed at EuXFEL of laser induced dynamics on water-filled capillaries with micrometer-scale spatial resolution sampled at 1.13 MHz (Fig. 1). This work opens up new possibilities for the characterisation of MHz stochastic processes on the nanosecond to microsecond time scales with object velocities up to a few kilometers per second and possibility to obtain 3D information per one pulse with sampling rate up to 4.5 MHz and photon energies up to 25 keV at EuXFEL.

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# Nucleation dynamics of skyrmion lattice from magnetic fluctuations phase

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Magnetic skyrmions are topological quasi-particles with diameters down to a few nanometers. These spin structures are attractive as information entities for spintronic applications, in particular for the realisation of current-driven magnetic shift registers, so-called racetrack memories. Generation, transport and annihilation of skyrmions are fundamental operations in this context. The non-trivial topology characterising skyrmions is believed to enhance their stability. However, despite the expected conservation of topological charge, skyrmion creation and annihilation through topological switching can be induced via field, current, or optical excitation. Yet, the mechanism and dynamics of the topological transition leading to a nucleation of skyrmions has remained unresolved. Here, we reveal the physics of ultrafast laser-induced topological switching by time-resolved X-ray scattering combined with atomistic simulations. Single-shot-resolved experiments at European XFEL allow us to track the magnetic correlation length and size of skyrmions nucleated in a short-range ordered lattice.

We find that skyrmion formation is a two-step process. First, the optical heat pulse induces a topological fluctuation phase where enough energy is available for atomistic spin-flip transitions. Subsequent to this nucleation step, micromagnetic energies lead to the collapse of antiskyrmions and coarsening of skyrmions, which freeze into a short-range ordered array with a controllable density upon rapid cooling. This ultrafast and controlled generation of topological charge paves the way towards new devices based on topological opto-spintronics.

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# Femto-second holographic X-ray imaging with FEL pulses of laser-induced cavitation bubbles

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Small transient or strongly driven cavitation bubbles in liquids exhibit a range of interesting nonlinear effects, from violent collapse and shockwave emission, sonoluminescence, and chemical reactions. For well-controlled experiments on cavitation bubbles, ultra-fast laser pulses are commonly used, which seed cavitation bubbles by a transition from a laser-generated plasma to a hot, compressed bubble nucleus, and finally to an expanding gas and vapour bubble in the liquid environment. This transition from the plasma to a bubble, the plasma growth, subsequent cooling of the plasma and generation of waves in the medium, as well as the precise states of matter in the bubble remain elusive. Apart from fundamental aspects of non-equilibrium physics, these processes are also relevant for applications such as laser surgery. More generally, cavitation effects are relevant for many more applications such as ultrasonic cleaning, and sonochemistry. For several decades, the main tool to study bubble dynamics has been optical imaging, with up to 100 million frames per second by high-speed CCD cameras. However, due to the small scales and the fast dynamics, imaging of the bubble interior and its environment remains a huge challenge. Nanosecond time resolution and sub-micrometer spatial resolution are required to follow the motion of the phase boundary and the dynamics of the bubble interior.

Coherent imaging with X-ray free-electron laser (XFEL) pulses now has enabled a quasi-instantaneous high resolution structural probe of cavitation bubbles at different stages after seeding. These novel capabilities to investigate extreme states of bubble generation and collapse offer a complementary contrast to ultra-fast optical microscopy and may help to improve our basic physical understanding of these processes. In this work we demonstrate how micrometer-sized bubble states can be probed by coherent X-ray flash imaging. An infrared ns laser pump seeds the cavitation process, while the X-ray laser is used to image the bubble by in-line holography using a highly focused XFEL pulse. By forward modelling and iterative phase retrieval the X-ray holograms are analysed to extract density and pressure distributions of the cavitation bubbles in space and time. The experiment provides an insight in the dynamics of single individual bubbles, with parameters histogrammed for over 10000 individually probed bubbles.

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# Static High Pressure Experiments on European XFEL

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In recent years, the exploration of high pressure states of matter using X-ray free electron lasers (XFELs) has revolutionised our knowledge of materials' structure and phase at extremes. With these X-ray sources intrinsically pulsed on femtosecond timescales, such studies have to date largely employed dynamic compression, where extreme pressures produced by transient pressure waves, e.g. generated by an optical laser pulse, can be quickly probed. Together with corresponding developments in dynamic compression at synchrotron facilities, the exploration of high pressure structural properties of matter using dynamic compression has seen a period of remarkable growth.

Alternatively, static compression, wherein matter is compressed isothermally in pressure cells, has long been used at synchrotron facilities in the exploration of high pressure structural states. However, the coupling of static compression with next generation XFEL techniques has been slow to materialise, in part because many traditional static high pressure techniques lack any dynamic aspect for which pulsed X-ray radiation is immediately beneficial. However, there is increasing realisation of a wide range of dynamic measurements performed using static pressure cells that can benefit from intense XFEL radiation, some made possible only at these sources. Rapid XFEL measurements can also overcome problems that often hamper traditional static experiments, such as chemical contamination and containment failure. XFEL facilities are now moving to accommodate static compression experiments, most notably, the European XFEL.

The European XFEL's High Energy Density (HED) instrument is dedicated to the study of matter at extreme conditions (e.g. of temperature and pressure). At this instrument, a dedicated platform for high pressure experiments using static compression cells has been developed using diamond-based anvils (the so-called Diamond Anvil Cell, or DAC), using a special interaction chamber (IC2). Nominally transparent to hard X-rays (>10 keV photon energy), diamond anvil cells enable the hermetic enclosure of samples at pressures of millions of atmospheres, similar to conditions occurring in the deep interior of the earth. This platform enables XFEL exposure, excitation, and probing of high pressure samples, with sample state studied by X-ray diffraction and optical pyrometry, and further modulated by rapidly varying pressure and temperature using cutting-edge piezo-driven cells and pulsed optical laser heating.

The HED instrument opened to first users in 2019, with the first community-wide experiment using DAC techniques, performed with the involvement of over 70 scientists from 7 nations (the HED-DAC Collaboration), conducted in October 2019, following preliminary experiments at the Pohang Accelerator Laboratory's XFEL in S. Korea. The objective of the EuXFEL experiment was to explore how matter under pressure responded to hard X-ray (17.8 keV) radiation at MHz repetition rates, including X-ray heating, structural transformation, melting, and chemical reaction, in compressed materials ranging from metals such as iron to molecular insulators such as hydrogen. The serial XFEL exposures excited extreme states and processes while simultaneously providing a rapid snapshot of the sample transformations. In achieving conditions of pressure up to and exceeding one million atmospheres, temperature of thousands of Kelvin, and timescales (of order 1 microsecond) compatible with the study of equilibrium matter, the experiment closely replicated the conditions and materials states found deep within planetary interiors. These studies go beyond a 'diffract-and-destroy' strategy, with the experiments revealing diamond anvils and samples to be robust under XFEL radiation, even at higher irradiances which annihilate similar samples at ambient conditions.

This talk will present the facility design and experimental benchmarks achieved through these first experiments, with an outlook to the next generation of static high pressure studies at European XFEL. In summary, XFELs hold the possibility of providing unprecedented access to the structural and phase behaviour of extreme states of matter, with their potential has now been realised at European XFEL.

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# Elastic and inelastic X-ray scattering from isochorically heated carbon

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As one of the very first user experiments at the HED instrument of European XFEL, we have realised an experimental platform for precisely studying the dynamics of dense carbon plasmas using spectrally resolved X-ray scattering, reaching a significantly enhanced data quality compared to previous proof-of-principle experiments at LCLS [1]. Elastic scattering from tightly bound electrons is highly sensitive to the ionic correlations and can therefore determine ultrafast changes in the ionic structure [2,3]. At the same time, inelastic scattering from free electrons gives direct access to the energy distribution of the electrons, from which the degree of ionisation and an average electronic temperature can be inferred [4]. Via inelastic scattering from bound electrons, we can accurately resolve the ionisation K-edge which provides the corresponding ionisation energy and thus the ionisation potential depression which, for dense plasma, is an area of very active scientific debate. Moreover, inelastic scattering from collective electron fluctuations can provide an additional constraint on the electronic temperature and ionisation. Finally, applying the 4-bounce monochromator, we have demonstrated the applicability of X-ray Raman spectroscopy as a highly promising diagnostics for electronic structure of dense plasmas, in particular for rep-rated experiments that will soon be enabled by the HIBEF infrastructure.

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# FLASH – today and tomorrow – status report and future plans

Martin Beye for the FLASH team

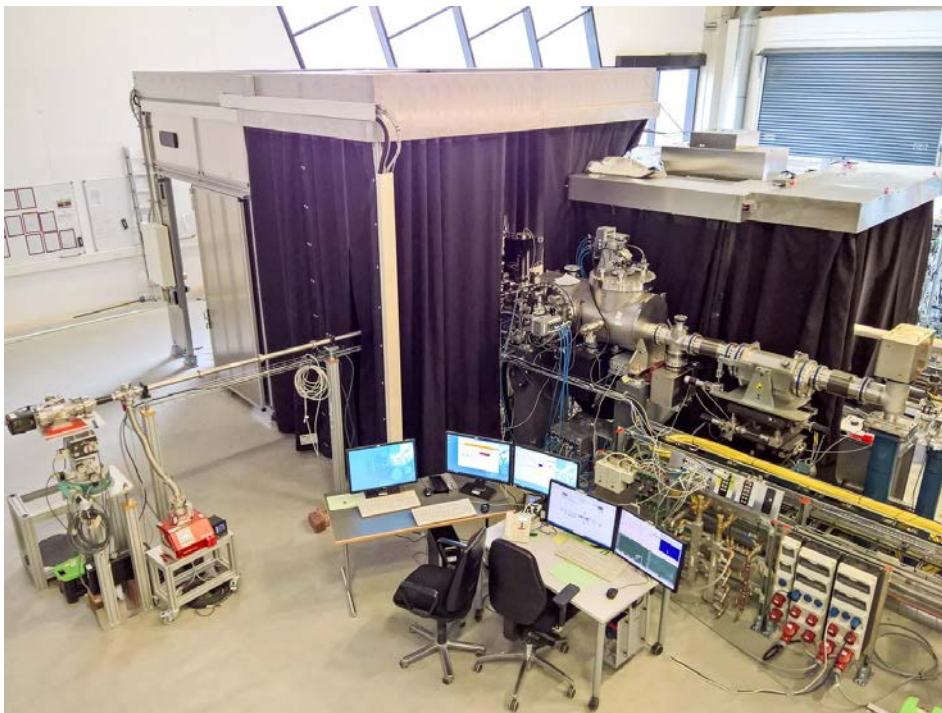
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In 2019, FLASH has been operated for a record high of about 4600 hours to deliver free-electron laser (FEL) beam to users, yielding in total about 6400 hours of beam for FEL experiments thanks to about 40% of parallel operation of the two undulator lines FLASH1 and FLASH2. The machine uptime of 98% also reached a new peak. With the routine operation of the new pump-probe laser at the FLASH2 beamlines FL24 and FL26, the tunable undulators in the FLASH2 section can be fully exploited for time-resolved experiments that also demand continuous scans of the FEL wavelength.

At the new beamline FL21 at FLASH2, a setup for THz streaking is continuously improved and further standardised in order to diagnose FEL arrival time and pulse lengths routinely on a shot-to-shot basis in non-invasive mode. Beamline FL26 with the Reaction Microscope end station now comprises an HHG setup synchronised with the FEL for novel XUV/VUV pump-probe experiments, installed within a BMBF collaborative research project led by the Leibniz Universität Hannover.

In order to further enhance parallel operation of FLASH1 and FLASH2 along with improvement of the beam quality and the FEL parameter range, the FLASH2020+ project has made significant steps forward with the completion of the conceptual design report. It is planned to develop FLASH1 into a high repetition rate, externally seeded FEL with fully coherent pulses (and fully tunable undulators), while FLASH2 focusses on ultrashort pulses covering the full soft X-ray range up to 1keV photon energy including harmonics.

In the talk, I will give an update on the status of FLASH, review instrumental developments and present some selected science results. Furthermore, a quick overview of the planned upgrades within the FLASH2020+ project is given together with a description of the current status.



The FLASH2 beamline FL24 at DESY, providing tunable FEL focal sizes and a large laser tent for user-provided experimental setups. Next to the large tent is a separate smaller laser tent for independent pump-probe laser beam preparation and monitoring.

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# THz/XUV pump-probe experiments for studying local fields and dynamics at surfaces

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Intense THz fields can be used to excite specific low-frequency modes in condensed matter or drive confined currents in nano-structured arrays, paving the way for a new class of optoelectronic devices. At the same time, these fields are themselves strongly influenced by the interaction with solid surfaces and nanostructures. A THz pump - XUV photoemission probe experiment can in principle study both sides of this coin. During the THz pump pulse, photoelectron streaking can be used for the polarisation-sensitive reconstruction of all electric field components at dielectric and metallic surfaces [1]. Between pump pulses, the XUV photoelectron spectrum and angular distribution can provide information on the THz-induced structural dynamics of the studied system.

In a proof-of-principle experiment we have studied the system of CO molecules adsorbed on Pt(111) at the THz beamline of the FLASH free-electron laser, using both, a single crystal sample and ultrathin films with Pt(111) islands of the order of few 100 nm lateral dimensions grown on Si(111). Using a conventional hemispherical electron energy analyser with a two-dimensional detector, resolving kinetic energy and one momentum component, the electrical field components of the THz pulses perpendicular and parallel to the Pt(111) surface could be reconstructed [2]. As expected, the parallel component is completely suppressed on the Pt(111) single crystal sample due to metallic screening, while it persists on the nanostructured film sample. Electric field simulations of THz radiation incident on nanometer-sized metallic islands show strong local variations of both field components in close proximity of these islands which cannot be resolved in these experiments. The distance over which the emitted photoelectrons interact with the THz pulse limits the spatial resolution at which the electrical fields can be characterised. The attempt to resonantly excite a low-frequency frustrated translational mode of CO on Pt(111) by means of these pulses [3] was unsuccessful as the signature of the structural dynamics in the XUV-excited photoelectron angular distribution was below the detection limit due to the limited THz field amplitude. Our results nevertheless help to identify the parameters required for studying structural dynamics at surfaces by means of THz pump - photoemission probe experiments.

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# Distorting atoms – The nonlinear driving of atom-specific transitions with intense XUV light

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With ultrafast XUV transient absorption spectroscopy, carried out in Fraunhofer-type transmission geometry by directly measuring the attenuated light, one is sensitive to both the linear and nonlinear XUV-optical dipole response of the electron dynamics in the local vicinity of an atom, enabling a direct view into the bound-state dynamics of excited electrons.

In this talk, we will present new results of direct XUV nonlinear effects in both helium [1] and neon [2] atoms. Intense XUV pulses from the free-electron laser (FEL) in Hamburg (FLASH) are tuned to photon energies of 60 eV and 50 eV, respectively, for the helium and neon absorption targets. The pulse energy ranges up to multiple ten  $\mu\text{J}$  with a photon fluence of several  $\text{J}/\text{cm}^2$  in the interaction volume. Depending on the stochastic substructure of the FEL pulses, intensities up to  $10^{15} \text{ W}/\text{cm}^2$  can be reached with these parameters.

With increasing XUV intensity, we observe a significant change of the asymmetric Fano line-shape of the strongly driven  $1s^2 - 2s2p$  two-electron transition in helium to a more symmetric absorption line at 60 eV photon energy [1]. Supported by a quantitative model we show how transient strong-XUV-field-induced energy shifts are directly encoded into the shape of the resonant absorption profile. The model also predicts an inversion of having more population in the upper  $2s2p$  state than in the lower  $1s^2$  ground state during a sizeable fraction of the 17 fs autoionisation lifetime.

For the case of neon, the XUV intensity is high enough to generate a significant abundance of  $\text{Ne}^{2+}$  ions within the target volume through the absorption of two photons at 50 eV. The  $\text{Ne}^{2+}$  ions are identified via  $^3\text{P}-^3\text{D}$   $2p-3d$  spin-orbit multiplet transitions within the measured XUV absorption spectrum. Depending on the XUV intensity, we observe 10-meV-scale spectral shifts of these lines due to the ac-Stark effect [2]. Furthermore, a few-femtosecond coherence enhancement through plasma-induced diffraction in the neon target is observed in the data and reproduced by a model of the characteristic SASE (self-amplified spontaneous emission) temporal structure of the FEL pulses.

New insights into strong-XUV-field light-matter interaction can thus be gained, demonstrating the feasibility of quantum control of specific transitions characteristic to each atom. The results also pave the road towards site-specific quantum control of molecular dynamics and chemical reactions by using intense and ultrashort FEL pulses.

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# X-ray Lasers Shed Light on the Mysteries of Water

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Water is of extreme importance for our society and the key component of life as we know it but it is also of extraordinary interest due to its remarkable physical properties that differ from almost all other liquids. Deviation of water's properties from a simple liquid exists already in the ambient temperature regime and then becomes strongly enhanced upon supercooling. In particular the finding that the thermodynamic response and correlation functions appear to diverge towards a singular temperature estimated by power-law fits of about 228 K has led to several hypotheses about the origin of water's anomalous properties. One hypothesis to explain the apparent divergence is that there exists a liquid-liquid transition with a liquid-liquid critical point at rather high positive pressures. In this scenario the Widom line, defined as the locus of correlation length maxima in the P-T plane, emanates from the critical point as a continuation of the liquid-liquid transition line into the one-phase region and the divergence in the response functions is towards this line. The challenge is that the temperature  $T_s$  lies below the homogeneous ice nucleation temperature 232 K, a region of the phase diagram that has been denoted as "no man's land", since ice crystallization occurs on much faster time scale compared to the experimentally accessible time scale in a typical laboratory setting.

Here I will present how X-ray lasers can be used to probe the liquid in the deep supercooled water regime inside no-man's land. In particular I will discuss if a liquid-liquid transition, Widom line and a critical point exists in deep supercooled water causing fluctuations all the way up to ambient temperature.

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## Imaging nanostructures in superfluid helium droplets

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Helium droplets are intriguing media for investigating particle growth. The droplet serves as an individual cryostat where captured dopant particles move without friction and spontaneously assemble far-from equilibrium nanostructures. In this talk, we report on X-ray coherent diffractive imaging of nanostructures grown in free, single, rotating, superfluid helium-4 droplets with diameters ranging from 150 to 2000 nm. The data presented here are collected from experiments conducted at the Linac Coherent Light Source at SLAC and at the European X-ray Free Electron Laser. Different dopant particles with different interatomic or intermolecular forces of attraction are used to investigate the effect of chemical bonding on the formation and growth of these nanostructures. Since quantum vortices are known to be present in superfluid droplets, we will also comment on how their presence influences the instantaneous positions of the dopants and nanostructure formation. Ultimately, it is the intention of these measurements to develop a model for dopant aggregation in helium droplets and the possibility of controlling their growth.

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# Evidence of Extreme Ultraviolet Superfluorescence in Xenon

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Superfluorescence describes the spontaneous, collective decay of a macroscopic ensemble of excited atoms or ions which have been prepared in a population-inverted state. It results in the emission of collimated, highly intense radiation pulses. Observing superfluorescence in the extreme ultraviolet (XUV) and soft X-ray wavelength regimes is difficult because of the disparate timescales of two competing processes: the very fast Auger decay on the fs (or Coster-Kronig decays on sub-fs) timescale limiting the lifetime of inner-valence vacancies and coherences, and the comparatively long (ns) radiative transition times.

Here, we demonstrate XUV superfluorescence by focusing the FLASH free-electron laser (FEL) in a cell filled with Xe gas. The FEL photoexcites the 4d shell of Xe atoms that rapidly decay via various Auger channels, thus creating a long-lived population inversion within the n=5 shell (Auger pumping). On the timescale of 10 to 100 ps, a macroscopic polarization builds up in the medium, resulting in superfluorescent emission of several Xe lines in the forward direction. As the number of emitters in the system is increased by either raising the pressure or the pump-pulse energy, the emission yield grows exponentially over four orders of magnitude and reaches saturation. With increasing yield, we observe line broadening, a manifestation of superfluorescence in the spectral domain. Our novel theoretical approach, based on a full quantum treatment of the atomic system and the irradiated field, shows quantitative agreement with the experiment and supports our interpretation.

In a second experiment, we study the emission of an ensemble of Xe clusters photoexcited by the same FEL, in transversal (fluorescence spectroscopy) and forward direction. Despite the different nature of the medium, we observe amplification of the same emission lines in forward direction as in the gas phase, with strikingly different characteristics. The creation of a nano-plasma in the warm dense matter regime, characterized by fluorescence spectroscopy, adds dephasing via heating and collisions which results in spectral broadening and quenches the superfluorescence. However, as our theory and extensive numerical simulations suggest, this harsh environment also opens an additional pathway to create strong, laser-like emission: population inversion is created by electron-ion collisions and decoherence processes can be characterized by a phenomenological dephasing time in the range of 100 - 200 fs.

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# Transient magnetic scattering in thin Co/Pt multilayers upon femtosecond IR excitation

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The dynamic response of magnetic order to ultrafast external excitation is a fascinating field of modern research on magnetism. Optical probing at the femtosecond time scale allows the investigation of ultrafast magnetisation dynamics, including fundamental interactions between spins, electrons, and lattice degrees of freedom far from equilibrium. Despite the picosecond magnetisation dynamics, even for non-uniform states, has been successfully modelled with spatially averaged models, there is a growing understanding of the important role played by spatially-varying magnetisation. Particularly important is unravelling the non-equilibrium spin dynamics following laser excitation on the nanometer length scale where magnetic order emerges. Access to the nanometer length scale during the ultrafast processes has only recently been achieved thanks to the development of XFEL's and new detectors of scattered X-rays. So far, this opportunity has been implemented only in study of ultrafast dynamics of spatial magnetic fluctuations in ferrimagnets with perpendicular magnetic anisotropy. In the present work, we used XFEL to study spatially resolved ultrafast magnetic dynamics in ferromagnet that arises after femtosecond laser pumping.

The experiment was carried out at the SCS beamline of EuXFEL by resonant magnetic SAXS in transmission geometry with the use of DSSC detector. The photon energy was tuned to the L-edge of cobalt at 779 eV. A femtosecond IR laser with a wavelength of 800 nm was used for pumping. The main results were obtained on a (1.0 nm Co/1.2 nm Pt)<sub>6</sub> multilayered sample. The static SAXS pattern of the non-magnetised sample was dominated by the low-q third order scattering ring at  $q \approx 0.07 \text{ nm}^{-1}$  corresponding to the maze-like multi-domain structure with domain size of about 60 nm. A sufficiently strong IR laser pulse was shown to cause an instant femtosecond-fast decrease of the low-q scattering followed by a picosecond-fast recovery. This is a known fingerprint of the ultrafast demagnetisation by IR radiation melting the magnetic domain order. Remarkably, for the IR fluences above  $3.3 \text{ mJ/cm}^2$ , additional scattering on shorter length scales (at high  $q > 0.8 \text{ nm}^{-1}$ ) appeared a few ps after the IR pulse. The re-formation and growth of magnetic order proceeds over picosecond time scales with a velocity in the km/s range. When a strong saturating field of 350 mT was applied, both static and transient low-q magnetic scattering completely vanished while the high-q transient magnetic scattering remained visible at a much lower level. This proves the magnetic nature of the observed transient effects.

The influence of the pump fluence and consequent sample heating have been investigated as the sample did not completely recover long range domain order during the 1.8  $\mu\text{s}$  between the subsequent FEL pulses. This is an evidence of the quasi-static pulse-by-pulse increase of base temperature on the  $\mu\text{s}$ -timescale. As a consequence, the transient magnetic signal at large q being the highest during the first pumped frame, faded away as the system was heated and vanished after several FEL bunches.

To conclude, we have for the first time observed a very bright transient magnetic scattering taking place in thin Co/Pt multilayers upon femtosecond IR excitation. This transient scattering is coupled to the destruction of magnetic domain order and occurs shortly after on a few picosecond time scale.

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# PETRA III and future outlook - PETRA IV

Christian G. Schroer for the PETRA III/IV group

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PETRA III is DESY's brilliant synchrotron radiation source and is in operation since 2009. Also, in the past year, its active user community has performed many cutting-edge experiments and produced exciting scientific results. Some of these results will be highlighted in this presentation.

Since 2014 PETRA III has been extended, adding two new experimental halls and a number of new beamlines to the facility. Many of these beamlines have taken up user operation, others are currently in commissioning or under construction.



DESY plans to upgrade PETRA III to the ultra-low emittance source PETRA IV [1,2]. It will enable new groundbreaking studies in many fields of science and industry, such as health, energy, earth and environment, mobility, and information technology. Being diffraction-limited up to X-rays of about 10 keV, PETRA IV will be ideal for three-dimensional X-ray microscopy of biological, chemical, and physical processes under realistic conditions with highest resolution and sensitivity. In 2019, the conceptual design of the new facility was completed. In the next phase, the technical design will be developed.

[1] C. G. Schroer, et al., J. Synchrotron Rad. **25**, 1277–1290 (2018)

[2] PETRA IV Conceptual Design Report, DESY (2019), DOI: 10.3204/PUBDB-2019-03613

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# Structural insights into the multifunctional L protein of bunyaviruses

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Bunyaviruses are a diverse group of viruses distributed globally, causing severe human diseases, such as the Lassa fever. Therefore, several bunyaviruses are listed on the WHO R&D Blueprint, which has been established to enhance preparedness for future epidemics and urge for the development of medical countermeasures, such as antiviral drugs.

Bunyaviruses are RNA viruses with a single-stranded genome in negative polarity that infect cells and use the cellular metabolism to amplify. A key factor for bunyavirus genome replication and transcription is the large 250-450 kDa L protein, a multidomain and multifunctional viral protein. The L protein performs at least two different jobs: (1) amplification of the viral genome, a process referred to as genome replication, and (2) viral transcription, that is synthesis of viral mRNA which encodes information for the production of viral proteins at the host cell ribosomes. However, to access the cellular protein production machinery mRNA usually requires a specific modification – a cap-structure. As bunyaviruses do not possess enzymes to synthesise caps, they “steal” the cap-structures of cellular mRNA by a so-called cap-snatching mechanism. Cap-snatching involves both a cap-binding site, which binds to host capped mRNA, and an endonuclease, which cleaves the host RNA a few nucleotides downstream of the cap-structure. An RNA-dependent RNA polymerase then synthesises the viral mRNA using the capped host RNA fragment as a primer. The endonuclease and RNA-dependent RNA polymerase functions are located in different domains of the L protein. Even though bunyavirus endonuclease domains have been structurally and functionally well characterised, evidence for the second important protein activity for cap-snatching, the cap-binding function, was missing.

We used X-ray crystallography to determine structures of bunyavirus L protein fragments and were able to identify a cap-binding domain in bunyavirus L proteins. Structural comparison to the related influenza viruses, which share the cap-snatching mechanism as a strategy for viral mRNA synthesis, revealed striking similarities concerning the protein architecture despite a very low sequence similarity. The details of the cap-binding site however differ from that of influenza. In summary, the crystal structures we solved represent evidence for a cap-binding function in bunyavirus L protein, a new target for the development of antiviral compounds to fight bunyavirus infections.

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# Size induced Structural Changes in Molybdenum Oxide Nanoparticles

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Small particles often show atomic structures different from the bulk material counterparts. These nanoscale atomic rearrangements can be utilised to tune materials properties; however, the nanostructures also pose a challenge to conventional structural characterisation techniques due to the small domain size and disordered nature. Structural characterisation is a critical part of materials development which makes the continual development of better tools for characterisation of structure on the nanoscale an important step in reaching the full potential of nanomaterials.

We have studied the atomic-scale structural changes occurring in MoO<sub>2</sub> nanoparticles at the nanoscale. Bulk MoO<sub>2</sub> adopts a distorted rutile structure; however, significant changes in the powder diffraction pattern of sub-10 nm particles indicate a fundamental structural rearrangement. In recent years total scattering and pair distribution function (PDF) analysis has emerged as a method for reliably characterising the atomic structure on the nanoscale, as it allows a direct view of the interatomic distances in a nanostructure. Utilizing the intuitive nature of the PDF method, we found that the structural changes relate to defects in the arrangement of the [MoO<sub>6</sub>]-octahedra that make up the structure of MoO<sub>2</sub>, and the octahedra show a larger tendency towards edge-sharing in the small particles. Similar crystallographic defects are known from bulk structures, and a simple model of the nanostructured MoO<sub>2</sub> is developed by applying these structural descriptions.

To achieve synthetic control of the defects in the MoO<sub>2</sub>, we also studied the formation of MoO<sub>2</sub> *in-situ* using total scattering. In solution, molybdenum ions form a range of polyoxometalate ions, POMs, where [MoO<sub>6</sub>] units are arranged in large, closed-shell clusters. Upon synthesis these break down to form the MoO<sub>2</sub> structures, and the POM may be considered pre-nucleation clusters. The nature of the POM present in solution is highly dependent on solvent properties, temperature and pH. By utilising this, we alter the prenucleation cluster structure, and in this way control the synthesis product to obtain both the pristine and highly defected MoO<sub>2</sub> structure. The differences in the structure of the products are linked to distinct reaction pathways from the clusters to the final product.

The studies highlight the value of PDF for nanostructural characterisation and obtaining information on the chemistry of nucleation. Greater understanding of nanomaterials' structure and chemistry will help to further develop nanomaterials as solutions to various challenges to society.

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# **Investigating Amphiphilic Monolayers with Grazing - Incidence Diffraction and X-ray Fluorescence**

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Soft interfaces constituted by molecular assemblies in two dimensions play key roles in numerous technological applications and are major components of all biological matter, for example in the form of biomembranes. The understanding of important biological or technological processes involving such interfaces typically relies on detailed structural insight.

We use various synchrotron-based X-ray diffraction and X-ray fluorescence techniques for the comprehensive characterisation of amphiphilic layers in terms of in-plane structural organisation, density profiles, elemental distributions, surface charge, and specific interactions with ions.

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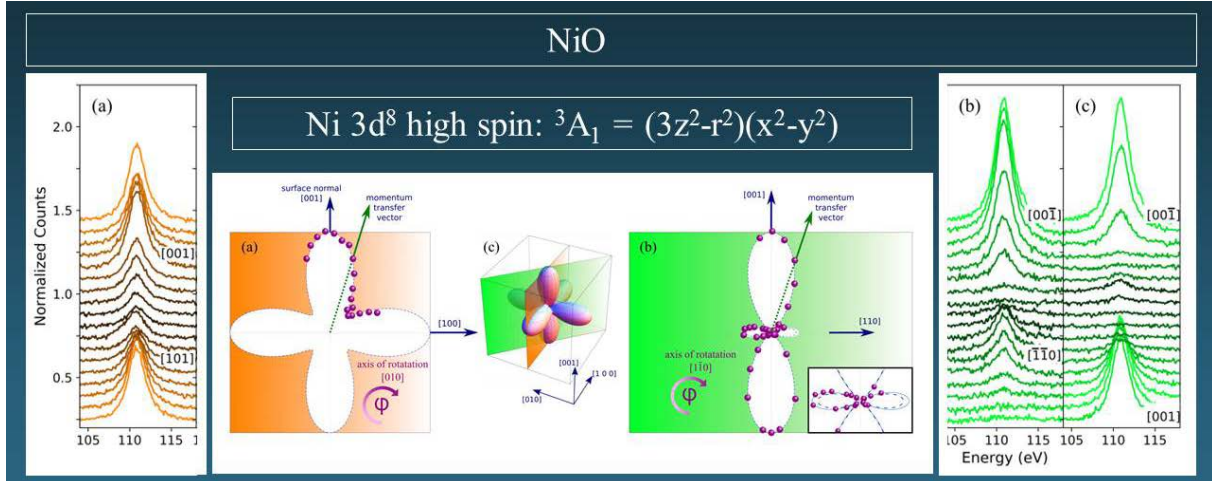
# Direct Imaging of Orbitals in Quantum Materials

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The search for new quantum materials with novel properties is often focused on materials containing transition-metal and/or rare-earth elements. The presence of the atomic-like  $d$  or  $f$  orbitals provides a fruitful playground to generate new phenomena. The intricate interplay of band formation with the local correlation and atomic multiplet effects leads to phases that are nearly iso-energetic, making materials' properties highly tunable by doping, temperature, pressure or magnetic field. Understanding the behavior of the  $d$  and  $f$  electrons is essential for designing and controlling novel quantum materials. Therefore, identifying the  $d$  or  $f$  orbitals that actively participate in the formation of the ground state is crucial. So far, these orbitals have mostly been deduced from optical, X-ray and neutron spectroscopies in which spectra must be analysed using theory or modelling. This, however, is also a challenge in itself, since *ab-initio* calculations hit their limits due to the many-body nature of the problem.

Here we developed a new experimental method that circumvents the need for involved analysis and instead provides the information as measured. With this technique, we can make a direct image of the active orbital and determine what the atomic-like object looks like in a real solid. The method,  $s$ -core-level non-resonant inelastic X-ray scattering ( $s$ -NIXS), relies on high momentum transfer in the inelastic scattering process, which is necessary for dipole-forbidden terms to gain spectral weight. To demonstrate the strength of the technique, we imaged the text-book example,  $x^2-y^2/3z^2-r^2$  hole orbital of the  $\text{Ni}^{2+}$  ion in NiO single crystal [1], see Fig. 1. We will present the basic principles of  $s$ -NIXS and its experimental implementation. We will also show how we can apply this technique to unveil the active orbitals in complex oxides such as  $\text{Ca}_3\text{Co}_2\text{O}_6$  [2], as well as to determine the orbital character in highly metallic systems such as elemental Cr, Fe, and Ni.



**Fig. 1:** Directional dependence of the spectral intensity associated with the dipole forbidden  $3s \rightarrow 3d$  transition directly maps the local hole charge distribution.

- [1] H. Yavaş, M. Sundermann, K. Chen, A. Amorese, A. Severing, H. Gretarsson, M.W. Haverkort, L.H. Tjeng, *Nature Physics* 15, 559 (2019); <https://doi.org/10.1038/s41567-019-0471-2>.  
[2] B. Leedahl, M. Sundermann, A. Amorese, A. Severing, H. Gretarsson, L.-Y. Zhang, A.C. Komarek, A. Maignan, M.W. Haverkort, and L.H. Tjeng, *Nature Communications* 10, 5447 (2019); <https://doi.org/10.1038/s41467-019-13273-4>.

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## **II Programmes Satellite Meetings**

# SATELLITE WORKSHOP - Photon Science



## Static Pressure Experiments at XFEL

27– 28 Jan.2020

DESY, FLASH Sem.R., Bldg. 28c

In October 2019 more than 70 scientist of the high pressure community from 7 nations collaborated in a community-assisted commissioning beamtime to develop a platform for high pressure experiments in the Diamond Anvil Cell at the High Energy Density (HED) Instrument of the European XFEL. The group benchmarked the capability of generating and probing extreme states using Diamond Anvil Cells, safely studying samples to pressures exceeding 1 Mbar. During the beamtime the group commissioned and tested the DAC setup in the 2<sup>nd</sup> interaction chamber (IC2) of the HED instrument in conjunction with a VAREX flat panel detectors in order to collect time-integrated diffraction images from samples exposed to femtosecond X-ray pulses at MHz repetition rates, to experimentally explore some crucial aspects of XFEL DAC science such as e.g. diamond stability and X-ray heating using 17.8 keV XFEL. In this workshop we will discuss not only the our findings from the October experiment but also give an overview of all DAC at XFEL experiments as well as the plans for the near future for DAC work at HED in IC2 and IC1.

Organisers: H. P. Liermann and Z. Konopkova

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### PROGRAM (27 Jan. 2020)

13:00	Welcome	C. Strohm	DESY
	<b>Session 1: Introducing DAC at XFELs Experiments</b>		Chair: Z. Konopkova
13:05	DAC Diffraction Experiments at XFELs: New Opportunities	H. P. Liermann	DESY
13:30	First DAC Experiments at PAL	A. Coleman	LLNL
13:55	Probing the electronic spin crossover in Fe-compounds at HED: new frontiers for high pressure science using the EuXFEL	V. Cerantola	XFEL
	<b>Session 2: DAC Setup at IC2 of the HED Instrument</b>		Chair: C. Strohm
14:20	DAC Alignment and X-ray Diffraction Capabilities of the IC2 at HED (EuXFEL)	C. Prescher	DESY
14:45	SOP Temperature Measurements in IC2	Z. Konopkova	XFEL
	<b>Session 2: Diffraction and X-ray Heating of Metal Foils using 17.8 keV X-ray of the EuXFEL</b>		Chair: E. McBride
15:15	Metal Foil Array Measurements at very low Pressures	M. McMahon	Uni. of Edinburgh
<b>15:15-16:00</b>	<b>Coffee break and Posters (45 Min.)</b>		
16:00	Fe and Fe alloys Experiments	G. Fiquet	IMPMC
16:25	Ta Experiments	Z. Jenei	LLNL
16:50	Melting of Mo at high pressures induced by intense X-ray pulses	C. Prescher	DESY
17:15	Au Experiments from PAL and at EuXFEL	R. Husband	DESY
17:40	Thermally-induced, quenchable bcc Zr using the European XFEL	B. Sturtevant	LANL
18:05	Reaction of W with H evidenced by Eu-XFEL	J. Kim	Hanyang Uni.
18:30	Comparison of T estimates from X-ray data (EOS) and SOP	St. McWilliams	Uni. of Edinburgh
<b>19:00</b>	<b>End of the 1<sup>st</sup> day (self-payd dinner) TBD</b>		



## PROGRAM (28 Jan. 2020)

9:00	Announcements		Institution
	<b>Session 3: Future Proposed Experiments at the HED instrument</b>		Chair: St. McWilliams
9:10	Single shot heating experiments, using pulsed laser or X-ray, in the DAC for MHz diffraction.	G. Morard	IsTerre
9:20	X-ray Heating of low-Z Materials at High Static Pressures	M. McMahon	Uni. of Edinburgh
9:30	Kinetics of structural phase transition in the dynamic-diamond anvil cell (dDAC): bridging static and shock compression	H. P. Liermann	DESY
9:40	Spin states of FeS and (Mg,Fe)O by X-ray emission at HED	Ch. Sternemann	TU Dortmund
<b>9:50-10:30</b>	<b><i>Coffee break and Posters (40 Min.)</i></b>		
10:30	Getting Ready for Proposed Experiments	C. Strohm, K. Appel	DESY
11:00	Close Out Discussion	St. McWilliams	Uni. of Edinburgh
11:30	Travel to EuXFEL for HED Satellite Meeting		



## User experience of data analysis at European XFEL

Tuesday 28 January 2020

DESY, CSSB lecture hall, Auditorium, Notkestraße 85, 22607 Hamburg

This community driven satellite workshop is focused on sharing user experience from users with users. The event is split into two short sessions on the topics of (i) online data analysis and (ii) offline data analysis and data reduction. This is complemented with opportunities to network through informal exchanges.

Both sessions of about 45 minutes are planned to start with three very brief presentation from users to kick start the discussions, who will use 3-slide presentations each to summarise the what, how and why of their specific data analysis at EuXFEL.

We invite all users to share their experience through participation in subsequent discussions. The remaining time is scheduled for questions and answers between presenters and audience. Future users are of course welcome to attend the event as well.

The emphasis of the event is on exchanging data analysis experience from using European XFEL to avoid duplication of effort, establish and share best practice, and for European XFEL to seek guidance on the community's wishlist for continued, improved and new services.

The workshop starts at 14:00 and concludes with an open ended coffee and networking session from approximately 15:40 onwards.

Organizers: Fabio Dall'Antonia,  
Hans Fangohr

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Tuesday 28 January 2020 – DESY, CSSB Lecture theatre (Bldg. 15)			
14:00	Welcome	Steve Aplin	European XFEL
14:10	Session 1 – online analysis		
		Valerio Mariani	CFEL
		Clemens Prescher	DESY
		Philipp Schmidt	European XFEL
14:55	Session 2 – offline analysis and data reduction		
		Filipe Maia	Uppsala University
		Oleksandr Yefanov	CFEL
		Michael Schneider	MBI Berlin
15:40	Coffee, networking and close		

# European XFEL Users' Meeting — Satellite meeting

## First experiments with a high-intensity short-pulse laser at HED/HIBEF

Mon. 27-28 January 2020 / Room: XTOB 1.01  
European XFEL, Holzkoppel 4, 22869 Schenefeld



The main goal of this workshop is to inform potential future users of the current development status of the high-intensity short-pulse laser commissioning at the HED instrument and discuss early user experiments. These include the High Intensity (~100 TW) laser (HIBEF/Amplitude) and the Pump-Probe laser (EuXFEL) systems. Summary and feedback to the previous 2017 workshop will be given. The workshop provides ample time for open discussion.

Organizer: Toma Toncian and Motoaki Nakatsutsumi  
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### Mon. 27 Jan 2020 – EuXFEL XTOB 1.01

13:30	<b>Welcome</b>	T. Cowan (tbd)	HZDR
13:40	<b>Summary of the last workshop “High Intensity Laser Matter Science at the HED Instrument at the European XFEL” in 2017. Desires and requirements.</b>	T. Toncian M. Nakatsutsumi	HZDR European XFEL
14:10	<b>Status of the instrument</b>	Chair: M. Nakatsutsumi	
14:10	Overview and status of the HED instrument	T. Preston	European XFEL
14:30	Status of the high-intensity 100 TW laser	T. Toncian	HZDR
14:50	Status of the online timing tool	J-P. Schwinkendorf	European XFEL
15:00	Status of the pump-probe (PP) laser	J-P. Schwinkendorf	European XFEL
15:10	<b>Coffee</b>		
15:40-16:45	<b>Roadmap towards standard setups</b>	Chair: T. Toncian	
15:40	Small angle X-ray scattering	M. Smid	HZDR
15:55	Polarimetry (recent XFEL experiment)	H-P. Schlenvoigt	HZDR / Jena
16:20	Phase contrast imaging (PCI) / nano-focusing	M. Makita	European XFEL
16:35	Fast sample scanner, robotic arm	M. Makita	European XFEL
16:45	EMP – current challenge and plans	S. Göde	European XFEL
16:55	<b>Small break</b>		
17:10	<b>Recent experiments</b>	Chair: A. Pelka	
17:10	Resonant SAXS experiment at LCLS	T. Kluge	HZDR
17:25	Small Angle X-ray Scattering on Rod Assembly Target at SACLA	M. Ota	U. Osaka, Japan
17:40	Overview of short-pulse laser experiments at LCLS	M. Gauthier/ C. Curry	LCLS
17:55	GISAXS experiment at SACLA	M. Nakatsutsumi	European XFEL
18:10	<b>Open discussion</b>	Chair: U. Zastra	
18:30	<b>Dinner Buffet at BeamStop Restaurant</b>		

### Tue. 28 Jan 2020 – EuXFEL XTOB 1.01

9:30	<b>Open discussion</b>	Chair: T. Toncian and M. Nakatsutsumi (tbd)	HZDR European XFEL
	Preparation for the first-day experiments		
	Community proposal		
11:30	<b>Final remarks, closing of the workshop</b>		
12:00	<b>Lunch at BeamStop Restaurant</b>		

# European XFEL Users' Meeting — Satellite meeting

## Chemical Dynamics Opportunities at the Scientific Instrument FXE



28 January 2020

European XFEL, Holzkoppel 4, 22869 Schenefeld and  
DESY, CFEL SemR I-III, Notkestraße 85, 22607 Hamburg

### Abstract:

The Femtosecond X-Ray Experiments (FXE) Instrument has recently taken large steps towards experiments for time-resolved x-ray emission (XES) and wide-angle scattering (WAXS) studies. The instrument can now host experiments, which demand an unprecedented high average flux and signal quality, possible due to the MHz delivery rate of 2-4 mJ X-ray pulses. The current status of the FXE will be given together with its upcoming capabilities.

This workshop seeks to bring together the scientific community aiming to exploit this instrument for chemical dynamics research benefiting from the spin and electronic sensitivity delivered from XES data, and from structural dynamics studies exploiting WAXS at up to 20 keV. The workshop will cover variety of topics in photochemistry, which can benefit for the simultaneous determination of coupled electronic and geometric transient structure changes on femtosecond time scale.

Organizers: Christian Bressler  
Wojciech Gawelda  
Dmitry Khakhulin

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Tuesday 28 January 2020 – DESY, CFEL Sem.R. I-III (Bldg. 99)			
09:00	<b>Welcome</b>	Sakura Pascarelli	European XFEL
09:15	FXE instrument update	Dmitry Khakhulin	European XFEL
09:45	Spin cross-over dynamics in biology and condensed matter	Majed Chergui	EPFL, Switzerland
10:10	Visualizing the ultrafast spin-dynamics in photoexcited Nickel tetrapyrroles	Sophie Canton	ELI-Alps, Hungary DESY, Germany
10:35	<b>Coffee break</b>		
11:00	Ultrafast X-ray spectroscopy to understand the photochemistry of base metal complexes	Matthias Bauer	University of Paderborn, Germany
11:25	Tracking coherent structural dynamics in solvated metal complexes	Martin M. Nielsen	DTU, Denmark
12:00	<b>Lunch at DESY Restaurant</b>		
13:30	Solving chemical processes dynamics with X-ray spectroscopy	Jacinto Sa	Uppsala University, Sweden
13:55	Luminescent 3d <sup>6</sup> and 4d <sup>6</sup> metal complexes made from Earth-abundant elements as alternatives to non-emissive Fe(II) compounds	Oliver Wenger	University of Basel, Switzerland
14:20	Tuning Ligand-Environments for the Stabilization of Iron Complexes in Oxidation States +I to +V, including Spin-Crossover in 4-Coordinate Fe(II)	Karsten Meyer	Friedrich Alexander University, Erlangen, Germany
14:45	Tracking reaction intermediates in catalytic reactions relevant to molecular artificial photosynthesis	Antoni Llobet	ICIQ, Spain
15:10	<b>Coffee break</b>		
15:30	Ultrafast, fast and slow structural changes of photoactive orange carotenoid protein during its photocycle	Eugene Maksimov	Moscow State University, Russia
15:55	Spinflip in chromium and vanadocomplexes	Katja Heinze	Johannes Gutenberg University, Mainz, Germany
16:20	Discussion Round	Christian Bressler	European XFEL
17:00	<b>Bus transport to European XFEL</b>		
17:30	Tour of FXE Instrument	all	
18:30	<b>Dinner at <i>BeamStop</i> Restaurant (at EuXFEL)</b>	all	



## MID Workshop: First year of operation and future developments

Mon 27 - Tue 28 January 2020 / Room: XHQ E1.173  
European XFEL, Holzkoppel 4, 22869 Schenefeld

The workshop is addressing the very first user experiments at the Materials Imaging and Dynamics (MID) instrument performed from March to November 2019. A status report of MID will be given together with selected presentations from user groups that span a diverse set of scientific topics, experimental techniques, and beam parameters. New equipment arriving at the instrument in 2020 will be discussed, e.g. a synchronized optical fs laser for pump-probe experiments and an X-ray split-delay line for XPCS applications. Together with developments of the source this will further broaden the scientific scope and strengthen the capabilities of MID.

Organizer: Anders Madsen

Contact: [anders.madsen@xfel.eu](mailto:anders.madsen@xfel.eu)

### Mon. 27 Jan 2020 – EuXFEL XHQ E1.173

<b>13:30</b>	<b>Welcome</b>	Sakura Pascarelli	European XFEL
<b>13:40</b>	MID status	Anders Madsen	European XFEL
<i>Session I. Chair: U. Boesenberg, European XFEL</i>			
<b>14:20</b>	Single pulse holographic imaging at MID	Johannes Hagemann	DESY
<b>14:55</b>	Evaporating laminar jets at XFELs for studies of crystal nucleation and growth in supercooled atomic liquids	Robert Grisenti	Uni. Frankfurt
<b>15:30</b>	Wavefront characterization using ptychography	Benedikt Daurer	National Uni. Singapore
<b>16:05</b>	<b>Coffee break</b>		
<i>Session II. Chair: J. Möller, European XFEL</i>			
<b>16:25</b>	New emerging possibilities at MID	Jörg Hallmann	European XFEL
<b>17:00</b>	Detector challenges in fast XPCS experiments	Christian Gutt	Uni. Siegen
<b>17:35</b>	High intensity with extreme focusing	Saša Bajt	DESY
<b>18:10</b>	Discussion and wrap up		
<b>18:30</b>	<b>Dinner Buffet at BeamStop Restaurant</b>		

### Tue. 28 Jan 2020 – EuXFEL XHQ E1.173

<i>Session III. Chair: A. Zozulya, European XFEL</i>			
<b>9:30</b>	Ultrafast X-ray photon correlation spectroscopy using hard X-ray split-and-delay line at FELs	Wojciech Roseker	DESY
<b>10:05</b>	Time resolved Bragg coherent diffraction imaging and fluctuation spectroscopy of oxide thin films	Ian Robinson	BNL & UCL
<b>10:40</b>	Collective radiative processes induced by the interaction of XFELs with matter	Andrei Benediktovitch	CFEL
<b>11:15</b>	<b>Coffee break</b>		
<i>Session IV. Chair: A. Madsen, European XFEL</i>			
<b>11:35</b>	Probing inhomogeneous structural dynamics and dynamic heterogeneity with LCLS-II	Diling Zhu	SLAC
<b>12:10</b>	Discussion, feedback and summary		
<b>13:00</b>	<b>Lunch</b>		
<b>14:00</b>	MID instrument visit (optional)		



European XFEL Users' Meeting — Satellite meeting:  
**Current status and future completion at the HED  
 instrument and the HIBEF contributions**



28. Jan. 2020 / XHQ E1.173  
 European XFEL, Holzkoppel 4, 22869 Schenefeld

The half-day workshop on the HED instrument and the HIBEF User Consortium will take place in the large seminar room E1.173 at the European XFEL headquarter building in Schenefeld. You will hear status updates of different experimental setups, which came online in the last month, and perspectives of the HED instrumentation also in view of beamtime application for upcoming runs. After a coffee break, the second part of the afternoon will concentrate on HiBEF UC contributions with special emphasis on the High-Energy laser DIPOLE, which will be installed and commissioned in 2020, and diagnostic tools used in shock compression experiments. In addition, status of the TW laser and planned first commission experiments will be represented. We plan for a reception in the “BeamStop” in the evening.

Organiser: Ulf Zastrau, Carsten Baetz  
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**Tue. 28 January 2020 – EuXFEL XHQ E1.173**

**13:30-16:00 User operation at HED**

13:30	Status of HED in 2019	U. Zastrau	European XFEL
14:00	Resolving low-frequency structural dynamics at the HED scientific instrument	L. Wollenweber	European XFEL
14:20	Simultaneous high pressure and high temperature XES and XRD measurements at HED	J. Kaa	European XFEL
14:40	Focus characterization in IC 1	M. Makita	European XFEL

15:10-15:30 *Coffee break*

**15:30-19:00 General HIBEF UC assembly**

15:30	Status of the HIBEF project	T. Cowan	HZDR
16:00	Dipole	T. Butcher	STFC
16:20	HIBEF contributions from LANL	C. Bolme	LANL
16:40	New VISAR at LULI 2000	L. Meignien	LULI
17:00	XANES at XFELs	M. Harmand	IUPMC
17:20	High-precision x-ray polarimetry at HED	K.S. Schulze	HIJ
17:40	Summary of the High-Intensity Laser experiments workshop	T. Toncian	HZDR
17:50	Route map to first DIPOLE experiments	M. McMahon	Edinburgh

18:30 *Light dinner in Beamstop*



# 1st meeting of the European XFEL Spanish user community

Thursday 30 January 2020

DESY, EMBL SemR, Bldg. 48e, Notkestraße 85, 22607 Hamburg

**Abstract:** This meeting intends to gather for the first time the Spanish community of European XFEL users, current and prospective, to discuss and identify common scientific interests and research lines. The synergy with the existing national user facilities and research centers as well as the development of strategies to facilitate the access to EuXFEL will be discussed

Organizer: Manuel Izquierdo  
Wojciech Gawelda

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[wojciech.gawelda@xfel.eu](mailto:wojciech.gawelda@xfel.eu)

## Thu. 30 January 2020 – DESY, Building 48e EMBL Seminar room L202

14:00-14:05	<b>Welcome</b>	-	Spanish Government
14:05-14:15	<b>The Spanish Community at EuXFEL</b>	Robert Feidenhans'l	European XFEL
<b>Part I: Proposed experiments at EuXFEL</b>			
14:15-14:40	Simultaneous probing of electronic correlations and structural changes during the ultrafast photodissociation of manganese carbonyl in solution	Luis Bañares	Universidad Complutense Madrid
14:40-15:05	Perspectives for Macromolecular Crystallography at X-ray Free Electron Lasers	Jose Martin-Garcia	Arizona State University
15:05-15:30	Time dependent atomic physics with non-thermal electron population for isochorically heated matter	Pedro Velarde	Universidad Politécnica Madrid
15:30-15:55	Stimulating the signal of Atom Mixing induced by Majorana neutrinos	Alejandro Segarra	Instituto Fisica Corpuscular Uni-Valencia-CSIC
15:55-16:10	Coffee Break		
<b>Part II: Scientific perspectives</b>			
16:10-16:35	Attosecond core-level spectroscopy - lightwave driven dynamics in condensed phase	Jens Biegert	ICFO - Institute of Photonics Science
16:35-17:00	Attosecond molecular dynamics with XFELs, a theoretical perspective	Fernando Martin	Universidad Autonoma Madrid
17:00-17:25	Artificial Photosynthesis: From solution to surfaces	Rodolfo Miranda	IMDEA Nanoscience Madrid
17:25-17:50	Time-resolved photoemission spectroscopy at FLASH and EuXFEL	Kai Rossnagel	Universität Kiel & FS-SXQM, DESY
17:50-18:00	Short Break		
<b>Part III: Spanish Photon Science User Facilities</b>			
18:00-18:25	VEGA, the Spanish High Repetition Rate Petawatt System	Luis Roso	Spanish Center for Pulsed Lasers - CLPU
18:25-18:50	The art to understand dynamics	Klaus Attenkofer	ALBA Synchrotron
<b>Part IV: Discussion</b>			
18:50-19:10	Strategies to develop Spanish EuXFEL		
19:10	<b>Dinner at DESY Canteen (UM2020 reception)</b>		

# SATELLITE WORKSHOP - Photon Science



## Coherent X-ray scattering and imaging

30. Jan. 2020

CFEL I-III, Bldg. 99 &  
SemR FLASH, Bldg 28c

New coherent x-ray scattering techniques have been developed, implemented and exploited at several instruments of PETRA III. These instruments use forward or Bragg scattering geometries or apply nano-focusing capabilities as e.g. provided by the P10-GINIX (build by the group of Prof. T. Salditt).

This workshop aims to give a comprehensive overview of available research opportunities / activities employing coherent X-rays.

The first part of this satellite workshop will be shared with the "10th workshop on X-ray Nano-Imaging of Biological and Chemical Systems at PETRA III" and present highlight results of different imaging approaches. The 2nd half of the satellite workshop will present the current state of the P10 beamline followed by presentations covering recent research activities.

Organizers: I. Vartaniants,  
M. Sprung

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[michael.sprung@desy.de](mailto:michael.sprung@desy.de)

### PROGRAMME (Session I: CFEL I-III)

<b>Session 1: Nano-imaging and P10 workshop session</b>		<b>Chair: G. Falkenberg</b>	
13:00	Welcome & X-Ray Microscopy Today and at PETRA IV	Christian Schroer.	DESY / UHH
13:20	News from the Nanolab	Thomas Keller.	DESY
13:30	Sample cells for X-ray ptychography and nanotomography - towards operando chemical imaging of catalysts and functional materials	Thomas Sheppard	Karlsruhe Institute of Technology
14:00	Multi-scale tomography of heart tissue: from Cardiomyocyte to whole heart	Marius Reichardt	University of Göttingen
14:30	Revealing the organization of axonal bundles from synchrotron tomography using streamline tractography	Hans Martin Kjer	Technical University of Denmark
15:00	3D anatomy and spatial chemistry in animal-microbe symbioses – Correlative phase-contrast x-ray tomography, metabolite imaging and fluorescence microscopy	Benedikt Geier	MPI Marine Microbiology

15:30-  
16:00 **Coffee break (30 Min.)**

<b>Session 2: Opportunities @ P10</b>		<b>Chair: I. Vartaniants</b>	
16:00	News/Updates from P10	Michael Sprung/ Markus Osterhoff Hendrik Rahmann	DESY/ University of Göttingen University of Siegen
16:20	Dynamics of liquid-liquid phase separation in protein solutions studied by low radiation dose XPCS		
16:40	X-ray induced dynamics in oxide glasses probed at inter-atomic length-scales	Francesco Dallari	University of Trento/DESY
17:00	Evolution of the strain field in Pt nanoparticles during CO oxidation using Bragg coherent imaging	Maxime Dupraz	ESRF/CEA
17:20	Correlation between Conductivity and Structure revealed by AXCCA in PbS Nanocrystal Superlattices	Dmitry Lapkin	DESY
17:40	Structural study of a single Au grain mesocrystal by Coherent X-ray Diffraction Imaging	Jerome Carnis	DESY
18:00	PETRA IV coherence properties	Ruslan Khubbutdinov	DESY
18:20	Closing remarks	Ivan Vartaniants/ Michael Sprung	DESY

18:25 **End of the workshop**



## Central infrastructure for DESY Photon Science Scientific computing - update and future directions

30 Jan. 2020

SemR BAH1/BAH2, Bldg. 3

This satellite workshop addresses the increasing demand for cooperation between central IT and DESY Photon Science in the field of scientific computing. It will give an update on work done in the previous years, solutions and practices at DESY today, and future plans and directions to address coming challenges including the coming needs of PETRA IV

Organiser: Anton Barty, Martin Gasthuber, Andre Rothkirch Contact: martin.gasthuber@desy.de

### PROGRAMME

14:00	Welcome and Introduction	Martin Gasthuber	DESY
14:15	Infrastructure update/news	Sven Sternberg	DESY
14:45	Analysis Services & Tools	Frank Schluenzen	DESY
15:05	HiDRA update and new developments	Manuela Kuhn	

#### 15:30-16:00 Coffee break (30 Min.)

16:00	Real-time streaming data analysis using ASAPO	Sergey Yakubov, Tim Schoof	DESY
16:40	Machine Learning - ongoing and future projects	Frank Schluenzen, Philipp Heuser	DESY
17:20	Answers to collected questions & discussion		

#### 18:30 *End of the workshop*



## ECB Workshop

30.01.2020

Seminar room 3, Bldg. 1b

### Description of workshop

In 2019 high-pressure research at the Extreme Conditions Beamline (ECB, P02.2) has continue to evolve. Experiments in the dynamic Diamond Anvil Cell at high-P have become a standard technique and the development of the simultaneous high-P and -T dDAC technique has further matured. We have also made progress in the development of imaging capabilities of the beamline, as well as in the calibration our standard resistive heated DAC setup together with our external partners. Submicron focusing is also becoming more robust and finds more and more users for ultra-high-pressure experiments. During this satellite meeting we will present ongoing research from different internal and external groups at the ECB and give an outlook on ongoing and foreseen technical developments.

Organizer: H. P. Liermann

Contact: [hanns-peter.liermann@desy.de](mailto:hanns-peter.liermann@desy.de)

## PROGRAMME

			Chair: K. Glazyrin
14:00	<b>Session 1: Experimental Capabilities of the ECB</b> Status of the ECB and Outlook	H. P. Liermann	DESY
			Chair: H. P. Liermann
14:30	<b>Session 2: Experimental highlights</b> Multi-megabar diffraction studies at the ECB: toroidal DACs with submicron beam	E. Pace	Uni. of Edinburgh
15:00	Towards understanding kinetics on fast compression in the dynamic-DAC	R. Husband	DESY/LLNL
<b>15:00-15:30</b>	<b>Coffee break (30 Min.)</b>		
15:30	Radial diffraction in the dynamic DAC	L. Q. Huston	LANL
16:00	Time-resolved X Ray Diffraction experiments with a Resistively Heated dynamic Diamond Anvil Cell (RHdDAC)	A. Mendez	DESY/Uni. of Bayreuth
16:30	The "shocking" effects of dynamic compression and heating experiments on quartz	C. Otzen	DESY
17:00	Kinetics of Deformation at high Compression Rates using dynamic Diamond Anvil Cell.	Ch. Plueckthun	XFEL
17:20	Revisiting the spin state crossover in single crystal (MgFe)O at the regime of high resolution	K. Glazyrin	DESY
17:50	Crystal chemistry of Fe-rich bridgmanite at lower mantle pressures	J. Koemets	Uni. of Bayreuth
<b>18:20</b>	<b>End of the workshop</b>		



## High Energy X-ray Diffraction for Physics and Chemistry

Thursday, 30 January 2020

CFEL, SemR IV, Bldg. 99

High energy X-ray diffraction and scattering based techniques have a unique impact in physics, chemistry, and materials science. In particular, they enable complex in situ and operando experiments and the analysis of local disorder on an atomic scale. This workshop brings together experienced users, interested researchers, and beamline staff. We are going to present and discuss the current and future capabilities available at the high-energy beamlines P07-DESY and P21.1 as well as key experiments that demonstrate the potential of these technique

Organizers: Ann-Christin Dippel, Martin v. Zimmermann

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[martin.v.zimmermann@desy.de](mailto:martin.v.zimmermann@desy.de)

### PROGRAMME

#### 14:00 Session 1

14:00	Status High Energy X-ray Diffraction Station P07-DESY	Ann-Christin Dippel	DESY
14:30	Status Broad Band Diffraction Beamline P21.1	Oleh Ivashko	DESY
15:00	Phase transformations in the nanowires of thiourea precursor of copper sulfide	Abhisakh Sarma	DESY

#### 15:30-16:00 Coffee break (30 Min.)

#### Session 2

16:00	Spatially Inhomogeneous Competition between Superconductivity and the Charge Density Wave in $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$	Jaewon Choi	University of Zurich
16:30	In-situ and operando high-energy grazing incidence X-ray diffraction	Vedran Vonk	DESY Nanolab
17:00	Structure-property relations from thermal diffuse scattering	Björn Winkler	University of Frankfurt
17:30	Discussion		

#### 18:00 End of the workshop





## Interfaces in electro chemistry, corrosion and solution based self assembly

Thursday, 30. 01. 2020

SemR. 109, Bldg. 25b

The goal of this meeting is to elucidate the role of interfaces in the fields of electrochemistry, corrosion and solution based self assembly, with special focus on their investigation by state-of the art x-ray diffraction and spectroscopy, as well as complementary methods. The DESY NanoLab opens a new electrochemistry and liquid interfaces lab for DESY Photon Science users, which will be presented during the workshop. Among a number of invited talks, interested participants is given to opportunity to present their work.

Organisers: Andreas Stierle, Olaf Magnussen, Bridget Murphy

Contact: andreas.stierle@desy.de

### PROGRAMME

14:00	Introduction	Andreas Stierle	DESY, FS-NL
14:05	Operando Insight into Structure, Composition and Reactivity Correlations in the Electrochemical Reduction of CO <sub>2</sub>	Beatriz Roldan	FHI Berlin
14:35	Electrochemical surface science of platinum	Marc T.M. Koper	Leiden University
15:05	In-Situ Stability Studies of IrO <sub>2</sub> -based model Electrodes under OER Conditions	Herbert Over	Universität Gießen
15:45	The brightest Au(111) surface	Edvin Lundgren	Lund University
<b>15:30-16:10</b>	<b>Coffee break (30 Min.)</b>		
16:10	Observing Pt(111) under operando oxygen reduction and evolution conditions	Leon Jacobse	DESY FS-NL
16:30	Passive film on super duplex stainless steel and its electrochemical stability studied by synchrotron X-ray technique	Jinshan Pan	KTH Stockholm
16:50	Inspirations from interface and corrosion science: Strategies toward design of interface-controlled materials	Nadiia Mameka	HZG
17:20	Understanding liquid structure and dynamics interfaces at LISA	Bridget Murphy	Universität Kiel
17:40	In situ study of the formation mechanism of two-dimensional superlattices from PbSe nanocrystals	Oleg Konovalov	ESRF
18:10	Layer by layer growth of semiconductor thin films: an operando SXRD study	Francesco Karla	Diamond Light Source
<b>18:30</b>	<b>End of the workshop</b>		

# SATELLITE WORKSHOP - Photon Science

## Helmholtz-Zentrum Geesthacht GEMS Outstation: Materials Research and High Resolution Imaging

Thursday, 30 January 2020

DESY Auditorium, Bldg. 5

Helmholtz-Zentrum Geesthacht operates the research platform GEMS with an outstation at DESY, running beamlines and instruments with a focus on engineering materials research and high resolution imaging techniques. On the 2020 satellite meeting, the status of the HZG beamlines and future perspectives are reported and users will present recent research highlights.

Organisers: C. Krywka  
P. Staron

Contact: christina.krywka@hzg.de  
peter.staron@hzg.de

### PROGRAMME

<b>Session 1: Imaging</b>			
14:00	Imaging instruments at IBL, HEMS and MINAXS	Christina Krywka	Chair: C. Krywka Helmholtz-Zentrum Geesthacht
14:15	Multimodal assessment of biodegradable Magnesium-based implants in bone	Berit Zeller-Plumhoff	Helmholtz-Zentrum Geesthacht
14:40	X-ray phase contrast Tomography for studying the Central Nervous System	Michela Fratini	CNR-Nanotec, La Sapienza University
15:05	Combined Diffraction Tomography and Fluorescence Tomography for spatially mapping elements in biological fiber reinforced nanocomposites	Paul Zaslansky	Charité - Universitätsmedizin Berlin Department for Operative and Preventive Dentistry
<b>15:30 Coffee break</b>			
<b>Session 2: Diffraction</b>			
16:00	Status of the diffraction beamlines	Norbert Schell	Chair: L. Lottermoser Helmholtz-Zentrum Geesthacht
16:15	FlexiDS – In-situ studies of directional solidification	Camelia Gombola	KIT, Inst. f. Angewandte Materialien
16:40	Hot forging wire and arc additive manufacturing	Joao Pedro Oliveira	NOVA University of Lisbon, Dep. Mech. & Industr. Eng.
17:05	Residual stresses in friction surfacing of Ti and Al alloys	Gleb Dovzhenko	Helmholtz-Zentrum Geesthacht
<b>17:30 Final discussion</b>			



## Light-Matter Interaction: Recent Advances in Theory

Thursday, 30 January 2019

CFEL, SemR V, Bldg. 99

The meeting will comprise 6 talks on the respective theory advances in atomic, molecular, solid state physics, warm-dense-matter and plasma research. Participation will be open to all interested users of photon science facilities, attending the EuXFEL and DESY Photon Science Users' Meetings.

Organisers: Beata Ziaja-Motyka (Executive), Sang-Kil Son, Ralph Welsch & Robin Santra (CFEL-DESY Theory Group)

Contact: [beata.ziaja-motyka@cfel.de](mailto:beata.ziaja-motyka@cfel.de)

### PROGRAMME

14:00	'Welcome Address'	Beata Ziaja-Motyka	CFEL, DESY Hamburg
14:15	'Strong-field control in the XUV domain'	Ulf Saalmann	MPIPKS, Dresden
14:45	'Polaritonic chemistry and materials: changing properties of matter by engineering the photon vacuum'	Michael Ruggenthaler	CFEL, MPSD, Hamburg
15:15	'Electron decay mediated charge redistribution in clusters'	Kirill Gokhberg	Univ. of Heidelberg
15:45	<b>Coffee break (30 Min.)</b>		
16:15	<b>Session 2 (Chairman: Ralph Welsch, CFEL, DESY)</b>		
16:15	'Free electron degeneracy in collisional-radiative simulations'	Howard Scott	LLNL, USA
16:45	'Essentially Exact Molecular Dynamics with Quantum Chemistry and Machine Learning'	Alexandre Tkatchenko	Univ. du Luxembourg
17:15	'New insights into nonlinear optical response with x-rays'	Daria Gorelova	CFEL, DESY, Hamburg
	'Closing Remarks'		& Univ. of Hamburg
17:45		Robin Santra	CFEL, DESY Hamburg
18:00	<b>End of the workshop</b>		

# SATELLITE WORKSHOP - Photon Science



## High-pressure Science in the Large Volume Press at P61B

30.01.2020

SemR 456, Bldg. 25f

Studies on mm-sized samples at high pressures (and temperatures) in the Large Volume Press using *in situ* X-ray techniques are now possible at beamline P61B. In the first half of 2020, commissioning continues with a Ge-SSD and a double-objective X-ray microscope for energy-dispersive X-ray diffraction in the energy range of 30 – 200 keV with an unprecedented amount of photon flux. Efforts to eliminate characteristic Pb emissions (from shielding) and to reduce the background in the diffraction patterns from scattered X-rays are promising. Dedicated radiography (imaging) experiments in the LVP can be carried out using a 2 mm x 2 mm beam. A precise detector positioning system (built by Kohzu) will be delivered and installed in the period of April – May 2020. Following this, a second Ge-SSD will be added to the detection set up. The LVP is fully adapted for many different anvil/assembly set ups and can operate in 3 modes of compression, particularly to enhance the opportunity to conduct *in situ* rock deformation studies. During this dedicated satellite meeting for the LVP beamline P61B, beamline status, ongoing research and collaborative efforts will be presented. The meeting offers an opportunity for current and new users to meet with the beamline staff and with each other to discuss new research ideas for high pressure studies in the fields of Earth and Materials sciences and organic/inorganic Chemistry. P61B is joining the current call for proposals for beam time starting in II-2020.

Organisers: R. Farla, S. Bhat

Contact: robert.farla@desy.de

## PROGRAMME

### Session 1

			Chair: R. Farla
14:00 – 14:10	<i>Introduction</i>	R. Farla	DESY
14:10 – 14:35	<i>In situ X-ray observation study using a large-volume press at ultra-high-pressure and ultra-high-temperature conditions</i>	T. Katsura	BGI, Univ. of Bayreuth
14:35 – 15:00	<i>Materials landscapes development in alloys and nitrides using pressure, temperature, X-rays and precession electron diffraction</i>	G. Serghiou	Univ. of Edinburgh
15:00 – 15:25	<i>Crystal structure evaluation of novel binary and ternary high-pressure nitrides, synthesized in the LVP at P61B</i>	L. Wiehl	T. U. Darmstadt

### 15:30-16:00 Coffee break (30 Min.)

### Session 2

			Chair: S. Bhat
16:00 – 16:25	<i>Chemical interaction in the B-X ( X = S, Se, Te ) systems at high pressure and high temperature</i>	V. Solozhenko	CNRS, Université Paris 13
16:25 – 16:40	<i>High-pressure synthesis of jadeite-based ceramic composites and their mechanical and optical performance</i>	E. Kulik	Univ. Kiel
16:40 – 16:55	<i>Supra-solidus phase relations of Ca-Mg-carbonates and melting point of hydrous magnesite in the upper mantle</i>	M. Sieber	GFZ, Potsdam
16:55 – 17:20	<i>Status and development of beamline P61B</i>	R. Farla	DESY
17:20 – 17:30	<i>Concluding remarks &amp; questions</i>		
17:30 – 19:00	<b>Beamline tour &amp; discussions</b>		

19:00

*End of the workshop*

# SATELLITE WORKSHOP - Photon Science



## SAXS/WAXS/GISAXS User Workshop @ DESY

30.01.2020

CSSB lecture hall, Bldg. 15

Following the big success of the SAXS/WAXS workshop in recent years, this workshop addresses current and potential users of small-angle X-ray scattering at PETRA III. It is intended to present and discuss the status and perspectives of the current and future experimental facilities in this field at DESY and recent as well as planned user activities. It shall foster communication among the users and identify common interests

Organisers: Rainer Gehrke, Stephan Roth

Contact: [Stephan.roth@desy.de](mailto:Stephan.roth@desy.de)

### PROGRAMME

13:00	Welcome & Overview of current and future SAXS capabilities at PETRA III	Stephan V. Roth	DESY & KTH
	<b>Session 1: Biomaterials - Cellulose</b>		Chair: Stephan V. Roth
13:10	P03 Nanofocus Endstation: news, updates, perspectives	Anton Davydok	HZG
13:25	Status of Biological SAXS at the EMBL P12 beamline	Andrey Gruzinov	EMBL
13:40	Well-defined polymers and surface modifications	Linda Fogelström	KTH
14:00	Formation of joints during drying of cellulose	Torbjörn Pettersson	KTH
	<b>Session 2: Composite Materials</b>		Chair: Stephan V. Roth
14:20	Advances at P03/MiNaXS	Matthias Schwartzkopf	DESY
14:35	Scattering from materials under deformation - state of the art and perspectives	Konrad Schneider/ Adam Kiersnowski	IPF & TUDD
14:55	Bone quality during skeletal development: structural and compositional adaptations on the micro- and nanoscale	Kilian Stockhausen	UKE
15:15	Nano Grain Mapping: High resolution 3D X-ray diffraction microscopy using nano focused X-rays	Hergen Stieglitz	HZG
<b>15:35-16:10</b>	<b>Coffee break (35 Min.)</b>		
	<b>Session 3: Mapping in reciprocal space</b>		Chair: Matthias Schwartzkopf
16:10	Small Angle X-ray Scattering Beamline for Materials Research (P62): Status and Outlook	Sylvio Haas	DESY
16:25	The high-resolution diffraction beamline P08 - status & highlights	Florian Bertram	DESY
16:40	Soft Matter Confined in Nanopores: 3-D Reciprocal Space Mapping and Single-Pore Diffraction Experiments	Patrick Huber	TUHH
17:00	Active layer printing of hybrid solar cells with in situ GISAXS and GIWAXS	Volker Körstgens	TUM
	<b>Session 4: Surface control</b>		Chair: Matthias Schwartzkopf
17:20	Studying organic solar cells in operando with GISAXS and GIWAXS	Peter Müller-Buschbaum	TUM
17:40	Probing the drying and consolidation of a wet-spun nanocellulose fiber using scanning SAXS	L. Daniel Söderberg	KTH
18:00	Structure Induced Device Degradation in Quantum Dot Solar Cell	Wei Chen	TUM
<b>18:20</b>	<b>End of the workshop</b>		



## High-energy X-rays for Swedish Materials Science (P21.2)

30 January 2020

SemR. O1.030, Bldg 48f

High-energy synchrotron x-rays provides a powerful probe for materials characterization across materials science disciplines. In order to meet the requirements from the Swedish materials community and to complement the lower energy synchrotron x-ray facility MAX IV, Sweden has invested in the Swedish Materials Science beamline (SMS) P21 at PETRA III. P21.2 is setup for experiments combining diffraction and small-angle scattering or imaging, in particular in-situ and in-operando studies are emphasized. After the commissioning phase basic functionalities are provided and the first user run has been completed. The beamline status and experiences at P21.2 will be reported. This workshop is intended to bring together the research community interested in the current and future capabilities of P21.2.

Organisers: P. Hedström, F. Eriksson, T. Zhou, U. Lienert      Contact: [ulrich.lienert@desy.de](mailto:ulrich.lienert@desy.de)

### PROGRAMME

<b>Session 1: Beamline &amp; experiments</b>			
13:00	Status of the SMS inline branch P21.2	Ulrich Lienert	DESY
13:30	User presentation	Ru Peng	LiU
13:50	User presentation	Magnus Colliander	CTH
14:10	User presentation	Jinshan Pan	KTH
14:30	User presentation	Emmanuel Larsson	RISE
14:50	Presentation thin-film deposition and cutting interaction	Fredrik Eriksson	LiU
15:10	User presentation	Johan Gustafson	LU
<b>15:30- Coffee break (30 Min.)</b>			
<b>16:00</b>			
<b>Session 2: Community activities &amp; discussion</b>			
16:00	Center for X-rays in Swedish Materials Science	Peter Hedström	KTH
16:20	Open session and Discussion about activities to stimulate Swedish community	N.N.	
17:00	P21 beamline tour		
<b>18:30 End of the workshop</b>			



# SATELLITE WORKSHOP - Photon Science



## Satellite Meeting: X-ray absorption spectroscopy at P64/65

Thursday, 30 January 2019

SemR 4ab, Bldg. 1b

The two XAFS-beamlines P64 and P65 are in user-operation mode now for a few years. The satellite workshop is intended to give an overview about the current status of the beamlines, the associated projects, and results from different external user groups. Short- and long-term plans for instrumentation concerning experimental techniques and sample environments will be presented and discussed, as well as results from users' experiments. Present and future users are strongly encouraged to participate in this workshop and to discuss their options with the beamline staff.

Organisers: Edmund Welter, Wolfgang Caliebe

Contact: [edmund.welter@desy.de](mailto:edmund.welter@desy.de),  
[wolfgang.caliebe@desy.de](mailto:wolfgang.caliebe@desy.de)

### PROGRAMME

#### Session 1: Instrumentation

*Chair: Wolfgang Caliebe*

14:00	Status of P65	Edmund Welter	DESY
14:20	Status of P64	Wolfgang Caliebe	DESY
14:40	High Resolution hard X-ray Spectroscopy at PETRA III Beamline P64: Present and Future	Aleksandr Kalinko	Univ. Paderborn
15:00	Status and future of time-resolved techniques at P64	Vadim Murzin	Univ. Wuppertal
15:20	tba	Michael Knapp	KIT

#### 15:40 Coffee break

#### Session 2: Experimental Results

*Chair: Edmund Welter*

16:10	tba	Marion Louvel	Univ. Muenster
16:25	tba	Anselm Loges	Univ. Muenster
16:40	Defect Investigations by element-specific excitation of optical luminescence	Sergiu Levenco	Univ. Leipzig
17:00	tba	Rachit Khare	TUM
17:20	Hard X-Ray Spectroscopy of organometallic complexes @ P64 beamline	Michal Nowakowski	Univ. Paderborn
17:40	Studies of heterogeneous catalysts using QEXAFS-XRD combination at P64, and the high temperature setup at P65	Dmitry Doronkin	KIT

#### 18:15 End of the workshop



## Satellite Meeting: 10th Workshop on X-ray Nano-Imaging of Biological and Chemical Systems at PETRA III

Thursday, 30 January 2020

CFEL Bldg.99, CFEL I-III

The workshop gives attention to X-ray microscopy at various PETRA III beamlines with special emphasis on applications in biology and chemistry. Several scientific highlights are presented and recent methodological and instrumental developments at PETRA III beamlines and the DESY NanoLab are discussed. X-ray microscopy will greatly benefit from a future upgrade of PETRA into the ultra-low emittance source PETRA IV. Participants are encouraged to discuss future scientific opportunities.

Organisers: G. Falkenberg & C.G. Schroer

Contact: Gerald.Falkenberg@desy.de

### PROGRAMME

<b>Session 1: Nano-imaging and P10 workshop session</b>			
13:00	Welcome & X-Ray Microscopy Today and at PETRA IV	Christian Schroer	Chair: G. Falkenberg DESY/UHH
13:20	News from the Nanolab	Thomas Keller	DESY
13:30	Sample cells for X-ray ptychography and nanotomography - towards operando chemical imaging of catalysts and functional materials	Thomas Sheppard	Karlsruhe Institute of Technology
14:00	Multi-scale tomography of heart tissue: from Cardiomyocyte to whole heart	Marius Reichardt	Goettingen University
14:30	Revealing the organization of axonal bundles from synchrotron tomography using streamline tractography	Hans Martin Kjer	Technical University of Denmark
15:00	3D anatomy and spatial chemistry in animal-microbe symbioses – Correlative phase-contrast x-ray tomography, metabolite imaging and fluorescence microscopy	B. Geier	MPI Marine Microbiology
<b>15:30-16:00</b>	<b>Coffee break (30 Min.)</b>		
<b>Session 2: Nano-imaging workshop</b>			
			Chair: C.G. Schroer
16:00	Nano-imaging experiments with Multilayer Laue optics	Sasa Bajt	DESY
16:20	Soft x-Ray Fluorescence Nanoscopy with the AnImaX endstation for biomedical and environmental applications	L. Lühl	TU-Berlin
16:40	X-ray fluorescence analysis of metal distributions in cryogenic biological samples	A. Rosenhahn	Ruhr-Univ. Bochum
17:00	Optical microscopy-driven imaging control software with online data visualization	S. Van Malderen	U Ghent
17:15	Self-Absorption Correction for XRF-Tomography at P06	D. Brückner	DESY/Uni HH
17:40	Coupled Ptycho-Tomography	M. Kahnt	Max IV
18:00	Missing wedge tomography with deep learning	Xiaogang Yang	DESY
18:20	Closing remarks	Christian Schroer	DESY
<b>18:25</b>	<b>End of the workshop</b>		

### **III Poster Session Topics**

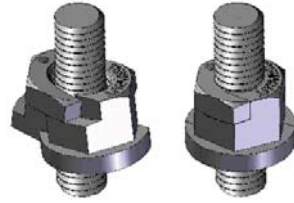
### III.1 Internal/Facility Poster

1. PETRA III: Advanced Applications of Synchrotron Radiation  
*O. H. Seeck, H.-C. Wille and C. Schroer*
2. PETRA III Beamline P61B: Science at Extreme Conditions Using the LVP  
*R. Farla, S. Bhat, S. Sonntag, A. Chanyshv, S. Ma, N. Nishiyama, N. Gaida, T. Ishii and T. Katsura*
3. P64 at PETRA III  
*W.A. Caliebe, M. Görlitz, A. Kalinko, V. Murzin, M. Naumova and A. Tayal*
4. PETRA IV – The Ultimate 3D X-ray Microscope  
*C.G. Schroer, S. Klumpp, R. Röhlberger, E. Weckert, R. Wanzenberg, I. Agapov, R. Brinkmann, W. Leemans and the PETRA IV project team*
5. DESY NanoLab  
*H. Noei, T.F. Keller, V. Vonk, R. Röhlberger and A. Stierle*
6. Sample characterization and laboratory support at the European XFEL  
*C. Deiter, H. Han, J. More, J. Makroczyová, J. Schulz, K. Dörner, K. Lorenzen, J. Adriano, M. Izquierdo, M. Kloos, M. Kitel, M. Vakili, R. Schubert and V. Bazhenov*
7. P62: Small Angle X-ray Scattering Beamline for Materials Research - SAXSMAT -  
*S. Haas, X. Sun, A. Conceicao and S. Pfeffer*
8. In Situ and Nano X-ray Diffraction beamline P23: status and prospects  
*D.V. Novikov, J. Raabe, A. Khadiev and K. Maksimova*
9. The Hard X-ray Micro/Nano-Probe beamline P06: Extending the energy range to 35 keV  
*G. Falkenberg, F. Seiboth, K.V. Falch, S.V. Malderen, A. Schropp and J. Garrevoet*
10. The High Resolution Diffraction Beamline P08  
*F. Bertram, R. Kirchhof, C. Shen, S. Volkov, A.B. Dey and G. Bussone*
11. Scientific instrument FXE  
*M. Biednov, D. Khakhulin, F.A. Lima, K. Kubicek, P. Zalden, A. Rodriguez-Fernandez, Y. Jiang, A. Galler, C. Bressler, P. Frankengerger, M. Knoll, T. Korsch, F. Otte, K. Boemer, T.K. Choi, M. Diez and W. Gawelda*
12. The SCS instrument: the soft X-ray beamline for spectroscopy and diffraction and coherent scattering  
*G. Mercurio, C. Broers, R. Carley, J.T. Delitz, N. Gerasimova, R. Gort, L. Le Guyader, L. Mercadier, A. Sorin, J. Schlappa, M. Teichmann, B. van Kuiken, A. Yaroslavtsev and A. Scherz*
13. Swedish Materials Science Beamline (SMS) at PETRA III: In-line branch (P21.2)  
*U. Lienert, S. Gutschmidt, T. Bäcker, Z. Hegedüs and T. Müller*
14. Coherence Beamline P10  
*F. Westermeier, V. Kartik, Z. Ren, R. Rysov, D. Weschke and M. Sprung*
15. Lab-Arena: The Development of Online Equipment Database of European and Worldwide Research Facilities  
*B.O. Postolnyi*
16. The Centre for Molecular Water Science (CMWS)  
*C. Goy, F. Lehmkuhler, M. Schnell and G. Grübel*
17. Resonant Scattering and Diffraction beamline P09 at PETRA III: Recent developments  
*S. Francoual, J.R.L. Mardegan, J. Sears, P. Bereciartua and J. Bergtholdt*

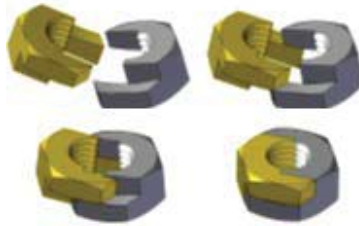


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18. Beamline P66 status report  
*A. Kotlov and I. Schostak*
19. The surface and beyond: Operando spectroscopy at beamline P22  
*C. Schlueter, Yu. Matveyev, P. Lömker, A. Gloskovskii, K. Ederer, I. Schostak and W. Drube*
20. Status of the Extreme Conditions Beamline (P02.2 and ECB)  
*H.P. Liermann, K. Glazyrin, A. Pakhomova, N. Giordano, M. Wendt and S. Wenz*

### III.2 Instrumentation and techniques

21. Status and future plans for the Diamond Anvil Setup (DAC) in IC2 at the HED instrument of the EuXFEL  
*H. P. Liermann on behalf of the HIBEF User Consortium and DAC user collaboration at HED of the EuXFEL*
22. A modular load frame system for applying compressive or tensile stress to materials  
*T. Dose, J. Brehling, H. Burmester, B. Eltzhig, J. Moosmann, E. Euchler and R. Bernhardt*
23. Operation of Photon Diagnostic Imagers at the European XFEL  
*A. Koch, J. Risch, W. Freund, M. Planas and J. Grünert*
24. Correcting wavefronts of multilayer Laue lenses  
*K.T. Murray, A.J. Morgan, M. Prasciolu, H.N. Chapman and S. Bajt*
25. Status and Outlook of the SAXS-CT sample environment at the SAXS beamline for materials research  
*A. Conceição and S. Haas*
26. X-ray standing waves method at the P24 beamline  
*M. Kamiński and M. Tolkiehn*
27. Compact Microfluidic Reactor for in situ Studies of Synthesis Stages  
*P. Medvedev*
28. Post-compression of picosecond pulses to four optical cycles  
*P. Balla, A. Bin Wahid, I. Sytceвич, C. Guo, A. Schönberg, A.-L. Viotti, L. Silletti, A. Cartella, S. Alisauskas, H. Tavakol, U. Grosse-Wortmann, M. Seidel, B. Manschwetus, T. Lang, F. Calegari, A. Couairon, A. L`Huillier, Cord L. Arnold, I. Hartl and C.M. Heyl*
29. Study of fast and ultra-fast time response of liquid-vapour interface by optical pump - X-ray probe technique  
*R. P. Giri, J. Warias, A. Sartori, B. Murphy and O. Magnussen*
30. Challenges and Lessons Learnt for Nanosecond Timing @ MID  
*M. Osterhoff, M. Vassholz, H. Hoppe, J. Rossello, R. Mettin, J. Hagemann, A. Schropp, C. Schroer and T. Salditt*
31. Updates from the GINIX instrument @ P10  
*M. Osterhoff, T. Salditt and M. Sprung*
32. Automation of experiments at the SPB/SFX instrument of the European XFEL  
*A. Round, R.J. Bean, J. Bielecki, K. Doerner, Y. Kim, H.J. Kirkwood, A. Legrand, R. Letrun, B. Manning, L. Lopez Morillo, G. Mills, N. Reimers, T. Sato, J. Schulz, C. Signe Takem, M. Sikorski, S. Stern, P. Thute, P. Vagovic and A.P. Mancuso*
33. Femtosecond 100 W-level OPCPAs from 800 nm to 2  $\mu\text{m}$   
*R. Riedel, M. Schulz, I. Grguras, T. Golz, J.H. Buß and M.J. Prandolini*
34. New AGIPD Detectors and Developments for the European XFEL  
*J. Becker, A. Delfs, R. Dinapoli, S. Fridman, P. Göttlicher, H. Graafsma, D. Greiffenberg, H. Hirsemann, S. Jack, A. Klyuev, H. Krueger, M. Kuhn, S. Lange, T. Laurus, A. Marras, D. Mezza, A. Mozanica, J. Poehlsen, S. Rah, B. Schmitt, J. Schwandt, O. Shefer-Shalev, I. Sheviakov, X. Shi, S. Stern, U. Trunk and M. Zimmer*

35. Smart\*Light – An Inverse Compton Source for Cultural Heritage  
*M. Alfeld, H.L. Casticum, P.H.A. Mutsaers, J. Dik, K. Janssens and O.J. Luiten*
36. X-ray measurements of bovine red blood cells in continuous flow  
*J. Burchert, G. Brehm, R. Graceffa, M. Burghammer and S. Köster*
37. An XUV and soft X-ray split-and-delay unit for FLASH2  
*M. Dreimann, S. Roling, I. Zadyraka, M. Kuhlmann, E. Plönjes-Palm, F. Wahlert, F. Rosenthal, M. Wöstmann and H. Zacharias*
38. Desk-top near edge soft X-ray absorption fine structure spectroscopy based on a laser plasma double stream gas puff target source  
*P.W. Wachulak, M. Duda, A. Bartnik, A. Sarzyński, L. Wegrzynski, M. Nowak, H. Fiedorowicz, A. Jančárek and L. Pína*
39. Classification of diffraction patterns in Single Particle Imaging experiments performed at XFELs using a Convolutional Neural Network (CNN)  
*A. Ignatenko, D. Assalauova, S.A. Bobkov, L. Gelisio, A.B. Teslyuk, V. A Ilyin, SPI consortium @ LCLS, A. Aquila and I.A. Vartanians*
40. Hanbury Brown and Twiss interferometry at SCS Instrument at European XFEL  
*R. Khubbutdinov, N. Gerasimova, G. Mercurio, D. Assalauova, L. Gelisio, J. Carnis, O. Gorobtsov, A. Ignatenko, Y.Y. Kim, R. Kurta, D. Lapkin, N. Mukharamova, M. Scholz, A. Scherz, A.P. Menushenkov and I.A. Vartanians*
41. FemtoMAX  
*A. Jurgilaitis, V. Pham, S. Checchia, H. Coudert-Alteirac, D. Kroon and J. Larsson*
42. Nanostructured diffractive X-ray optics from the Paul Scherrer Institut  
*F. Döring, A. Kubec and C. David*
43. A direct temperature measurement of resistively heated diamond using inelastic X-ray scattering  
*A. Descamps, B. Ofori-Okai, L. Fletcher, J.B. Hastings, O. Karnbach, D. McGonegle, C. Palmer, O. Humphries, J. Wark, G. Gianluca, U. Zastra, K. Appel, L. Wollenweber, T. Preston, C. Strohm, C. Plueckthun, A. Comley, A. Jenei, J. Eggert, R. Loetzsch, I. Uschmann, D. Senesky, S.H. Glenzer and E.E. McBride*
44. Harmonic lasing self-seeding at FLASH and the European XFEL  
*E. Schneidmiller, F. Brinker, W. Decking, B. Faatz, M. Guetg, M. Kuhlmann, S. Liu, D. Noelle, J. Roensch-Schulenburg, M. Scholz, S. Schreiber, M. Tischer, M. Yurkov, I. Zagorodnov, N. Gerasimova, G. Geloni, J. Gruenert, J. Laksman, Y. Li, J. Liu, S. Karabekyan, N. Kujala, Th. Maltezopoulos, I. Petrov, L. Samoylova, S. Serkez, H. Sinn and F. Wolff-Fabris*
45. Simulating wavefront propagation for a beamline with split-and-delay unit and compound refractive lenses at the European X-ray Free Electron Laser  
*V. Kärcher, S. Roling, L. Samoylova, A. Buzmakov, U. Zastra, K. Appel, M.V. Yurkov, E. Schneidmiller, F. Siewert and H. Zacharias*
46. Single-shot pulse-energy correlations between multiple devices at European XFEL  
*Th. Maltezopoulos, O. Brovko, F. Dietrich, W. Freund, A. Grebentsov, U.F. Jastrow, A. Koch, J. Laksman, J. Liu, M. Planas, A. Sorokin, K. Tiedtke and J. Gruenert*
47. Adaptive X-ray optics for time-resolved studies  
*V. Akkuratov, I. Eliovich, A. Targonskii, Yu. Pisarevsky and A. Blagov*
48. A Machine Learning Approach to XFEL Data Analysis  
*P. Vester*
49. Recent developments towards high-flux time-resolved & THz-SAXS experiments at the EMBL P12 BioSAXS beamline  
*M.A. Schroer, S. Schewa, C.E. Blanchet, A. Y. Gruzinov, I. Josts, S. Fiedler, H. Tidow, G. Katona, M. Roessle and D.I. Svergun*



50. Commissioning and first experimental observations of bent diamond spectrometer at MID instrument of European XFEL  
*I. Petrov, U. Boesenberg, J. Hallman, K. Kazarian, C. Kim, W. Lu, A. Madsen, J. Moeller, M. Reiser, L. Samoylova, M. Scholz, R. Shayduk and A. Zozulya*
51. First observations of heat load effects on cryo-cooled monochromator at European XFEL  
*I. Petrov, U. Boesenberg, M. Dommach, J. Eidam, J. Hallman, K. Kazarian, C. Kim, W. Lu, A. Madsen, J. Moeller, M. Reiser, L. Samoylova, M. Scholz, R. Shayduk, H. Sinn, V. Sleziona, A. Zozulya, X. Dong, J. Anton, S. Kearney and D. Shu*
52. URSA-PQ@FLASH: A mobile and highly flexible endstation for pump-probe electron spectroscopy at FLASH2  
*J. Metje, D. Mayer, F. Lever, M. Niebuhr, M. Robinson, A. Heuer, R. Squibb, R. Feifel, S. Düsterer and M. Gühr*
53. Laser-induced transient thermal gratings for pulse picker applications  
*D. Schmidt, R. Bauer and P. Gaal*
54. Deep Learning: New Approaches for the Investigation of Protein Dynamics via XPCS  
*S. Timmermann, H. Rahmann, A. Girelli, N. Begam, A. Ragulskaya, M. Reiser, C. Lovato, F. Westermeyer, M. Sprung, F. Zhang, F. Schreiber and C. Gutt*
55. Thermal diffuse scattering X-ray measurements on a metal-organic framework compound and on thiourea with high energy photons  
*J. Büscher, M. Stękiel, D. Spahr, W. Morgenroth, E. Haussühl, O. Ivashko, M. von Zimmermann, A.-C. Dippel and B. Winkler*
56. A hard X-ray Split-and-delay Unit for the High Energy Density Instrument at the European XFEL  
*S. Roling, V. Kärcher, D. Eckermann, K. Appel, S. Braun, P. Gawlitza, F. Siewert, U. Zastra, M. Dreimann, F. Wahlert and H. Zacharias*
57. Liquid Sample Delivery Solutions at the European XFEL  
*M. Vakili, L. Adriano, K. Dörner, H. Han, M. Kloos, J. Knoska, A. Mancuso, J. Makroczyova, M. Sawatzki, R. Schubert and J. Schulz*
58. X-ray multibeam ptychography  
*F. Wittwer, M. Lyubomirskiy, F. Koch, M. Kahnt, M. Seyrich, J. Garrevoet, C. David and C. Schroer*
59. Beamlines at PoFEL facility  
*K. Szamota-Leandersson, R. Nietubyć, J. Sekutowicz, P. Czuma, P. Krawczyk, J. Lorkiewicz, N. Palka, P. Zagrajek, P. Wachulak, K. Janulewicz, H. Fiedorowicz, J. Krzywinski, M. Terka, M. Staszczak and J. Szewiński*
60. Mobile instrumentation set-up for X-ray diffraction imaging applied at PETRA III  
*S. Haaga, M. Kabukcuoglu, S. Bode, D. Hänschke, E. Hamann, M. Zuber, T. Baumbach and A. Danilewsky*
61. Intensity Correlations in Radiographic Images  
*C. Niehaves and T. Salditt*
62. EUV Wavefront sensing at near field for characterizing a Schwarzschild objective  
*M. R. Lopez, M. Mehrjoo, B. Keitel, E. Plönjes, U. Zastra, D. Alj, L. Lu, G. Dovillaire and P. Zeitoun*
63. Compact hard X-ray split-and-delay line for studying ultrafast dynamics at free-electron laser sources  
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65. Time-resolved high resolution resonant inelastic soft X-ray scattering end station at the FLASH PG1 beamline  
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66. First Characterization of the Photon Beam at the European XFEL in July and 2017  
*V. Balandin, B. Beutner, F. Brinker, W. Decking, M. Dohlus, L. Froehlich, U. Jastrow, R. Kammerling, T. Limberg, D. Noelle, M. Scholz, A. Sorokin, K. Tiedtke, M. Yurkov, I. Zagorodnov, J. Liu, L. Samoylova, U. Boesenberg, W. Freund, J. Grünert, A. Koch, N.G. Kujala, T. Maltezopoulos, M. Messerschmidt, I. Petrov and H. Sinn*
67. Experience With MCP-Based Photon Detector at FLASH2  
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68. Femtosecond Temporal Multiple Diffraction in Single Crystals  
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*J. Sears, P.J. Bereciartua, M. Kusch, G.S. Thakur, K. Glazyrin, J. Geck, M. Jansen and S. Francoual*
70. High-speed pixel detector development  
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*M. Seyrich, L. Grote, F. Wittwer, M. Kahnt, D. Brueckner, R. Doehrmann, S. Botta, P. Wiljes, J. Garrevoet, D. Koziej and C. Schroer*
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79. Shock heating and Melting of Fe with an X-ray laser  
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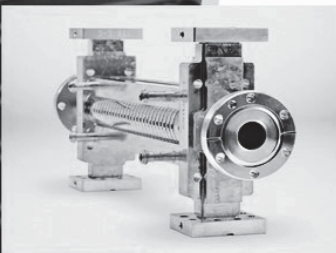
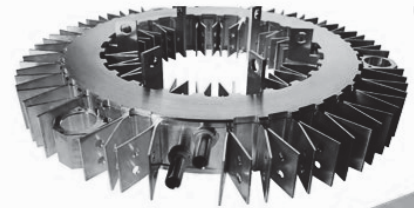
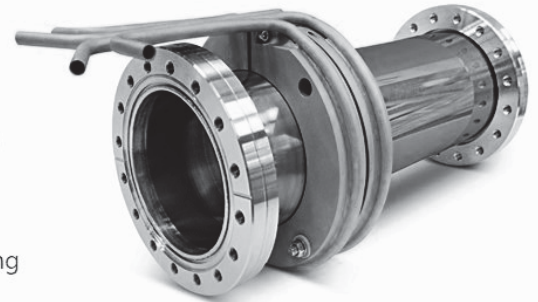
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### **III.3 Atoms, molecules, clusters, ions and plasmas**

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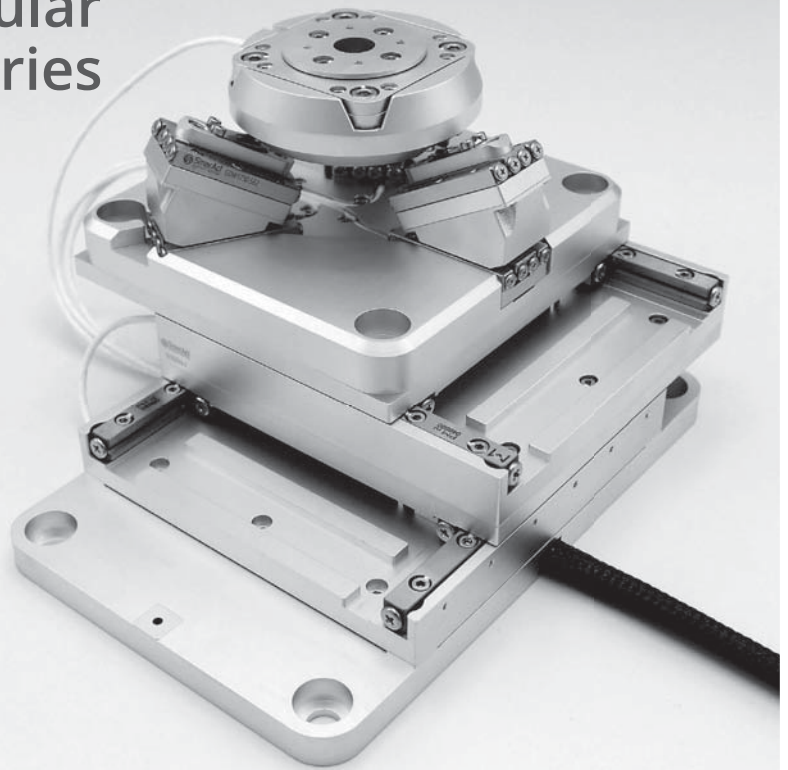
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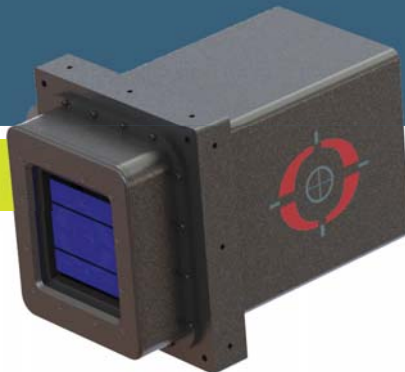
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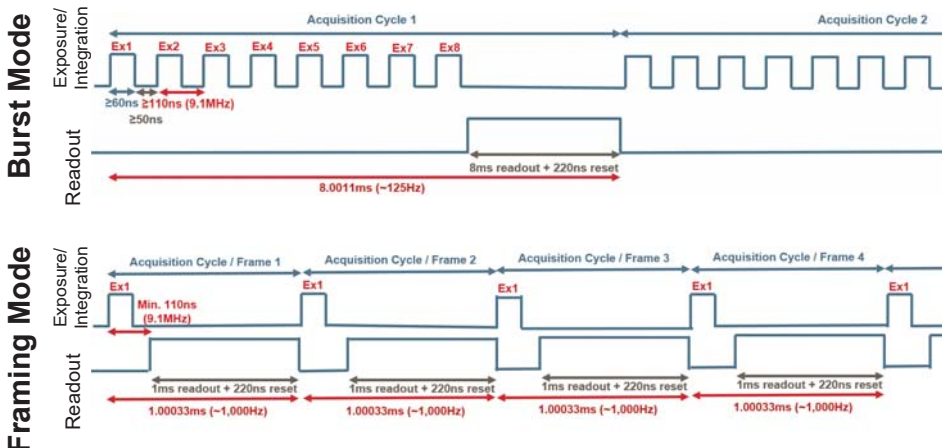


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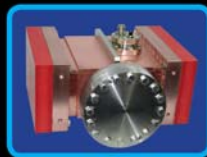
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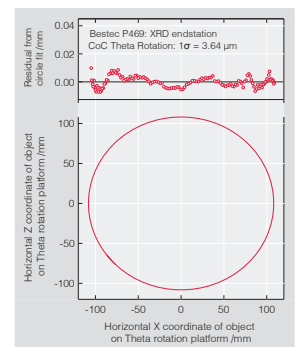
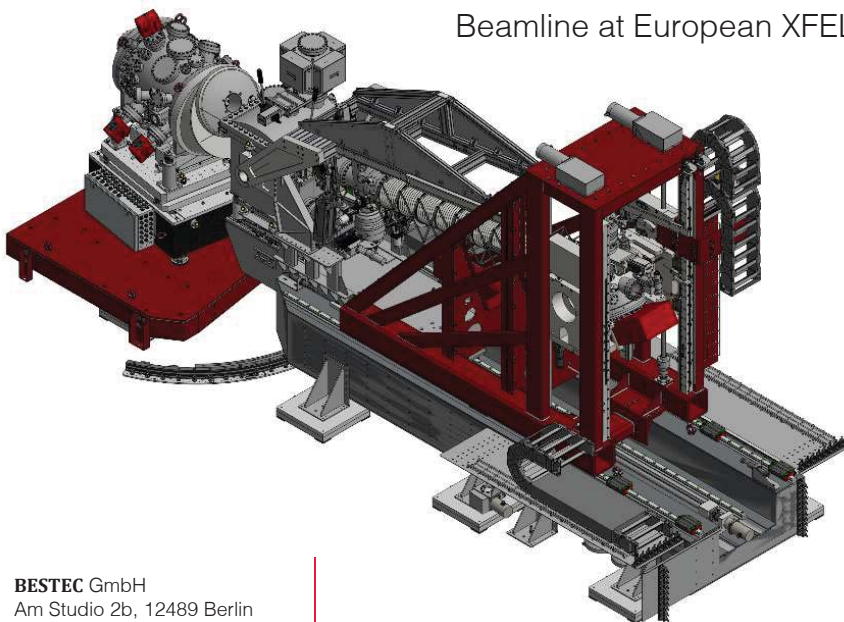
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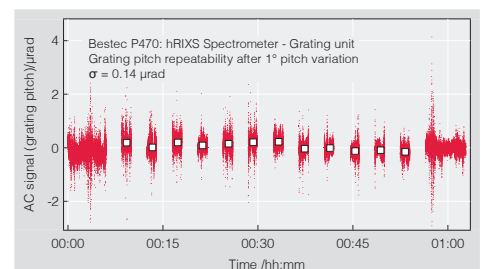
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- Wayforlight: the catalogue of European lightsources (C. Blasetti)
- Lightsources.org (F. Krawatzek)
- LEAPS (U. Krell)
- KFS - Komitee Forschung mit Synchrotronstrahlung (K. Griewatsch)
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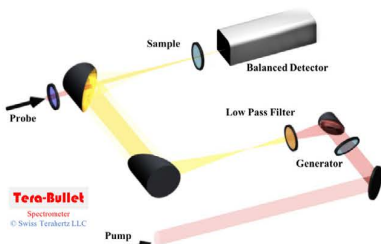
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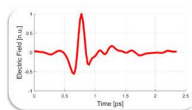
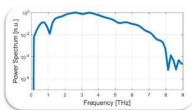


Technology of the world most intense THz source at affordable prices

### Tera-Bullet



- Intense THz spectrometer for nonlinear spectroscopy and electron acceleration
- Starting from 9k Eur



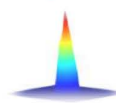
### RIGI uncooled micro-bolometer



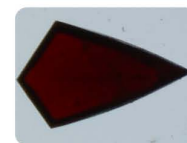
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- Sold with 1 year warranty
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- Active Area (> 29 x 16 mm)
- Array size (> 1M Pixel)
- Starting from 2.8 Eur

**Extremely sensitive: NEP/pixel < 1.5 pW/√Hz**

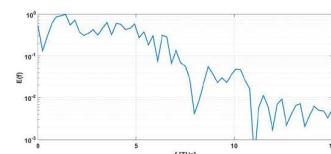
- Frequency: 4,6 THz
- Power: 0.6  $\mu\text{W}$
- Integration time: 50  $\mu\text{s}$
- Acquisition: Single shot



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- Operate at Ti:Sa, OPA, OPCPA and 1  $\mu\text{m}$  lasers
- Most efficient and affordable organic emitters
- Sold with 2 years warranty
- Up to 83 MV/cm THz fields (world record)
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pump

1% efficiency

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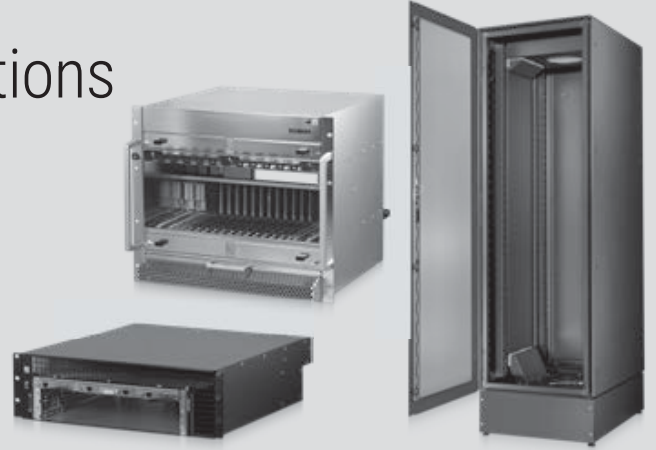


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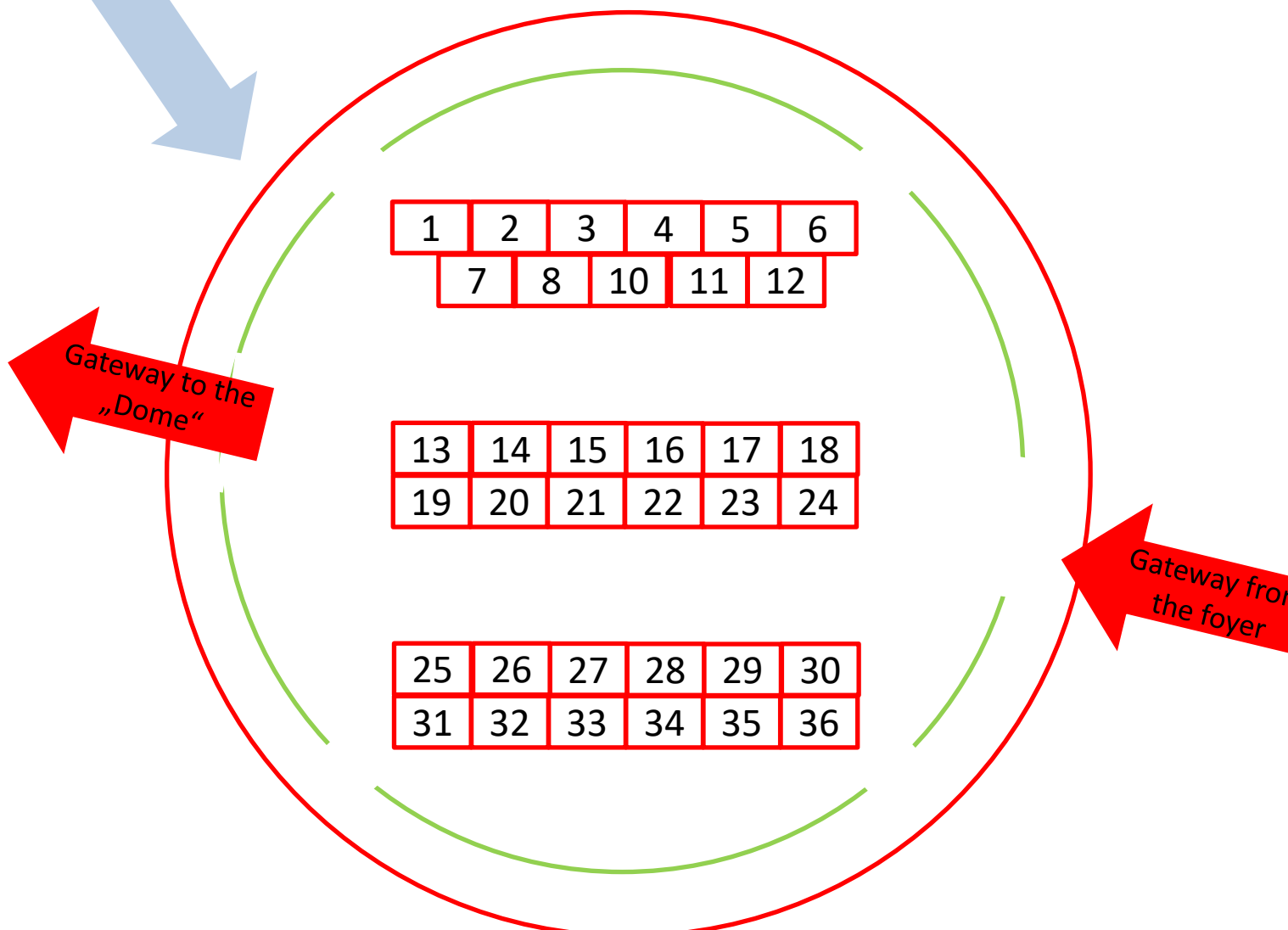
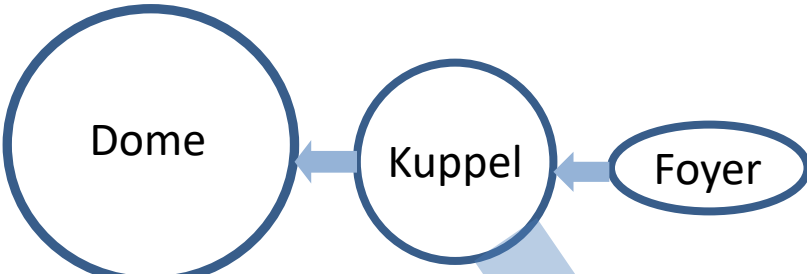
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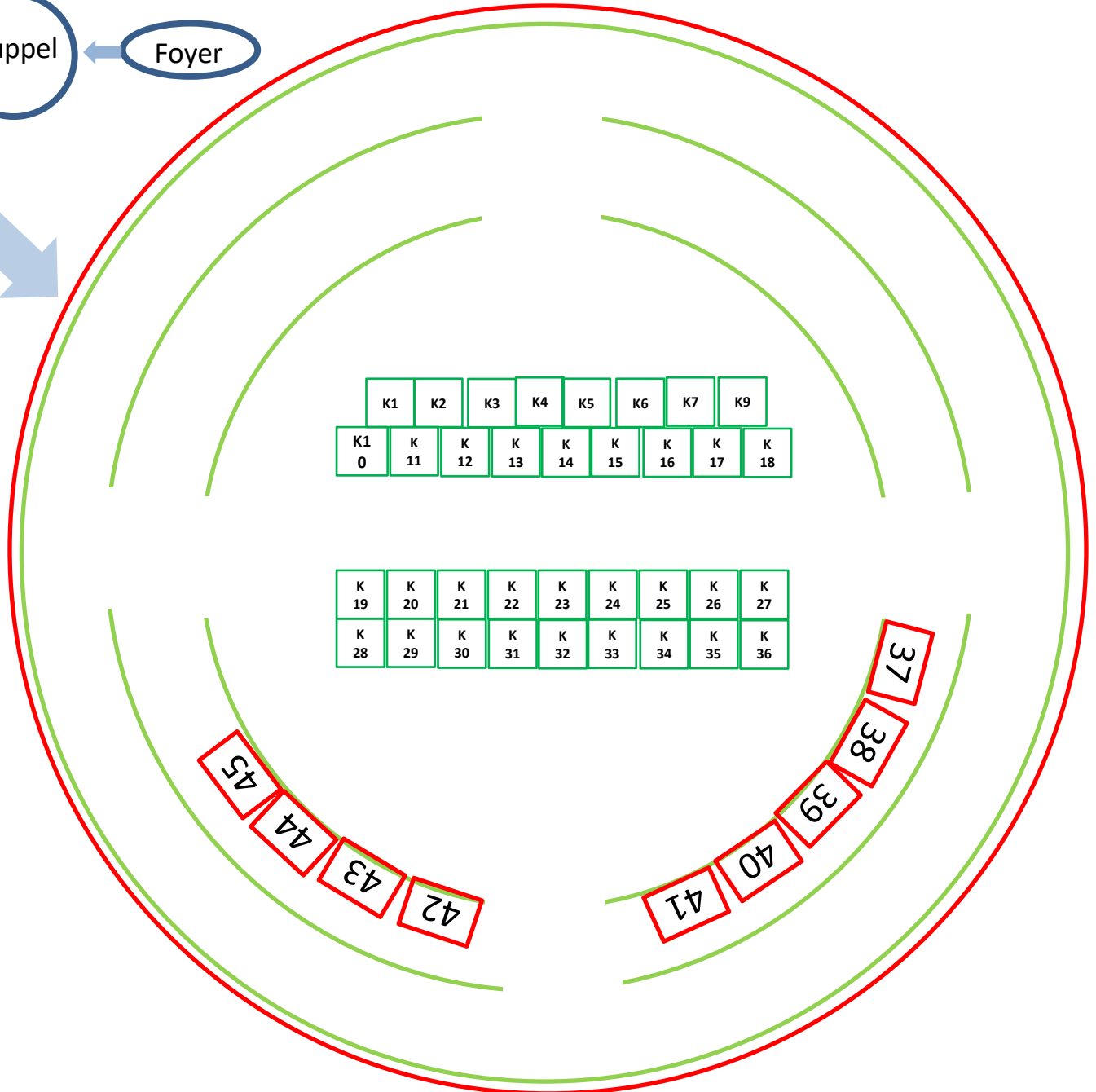
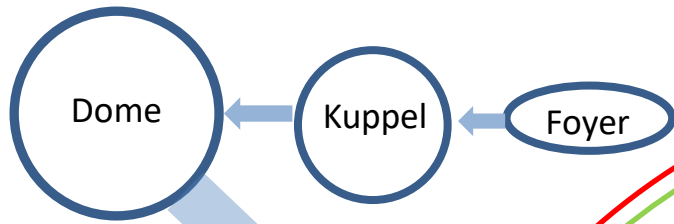


# Industry Exhibition and Poster Session

Location: Kuppel and Dome Hamburg Luruper Chaussee 30 – see Campus Map

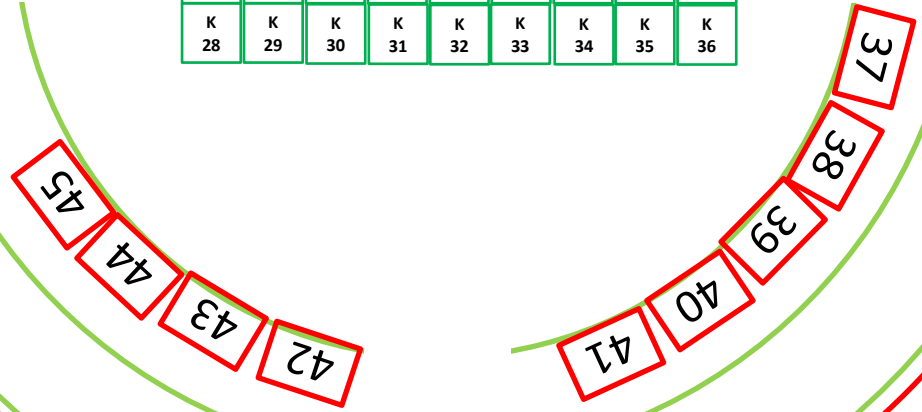


# Industry Exhibition and Poster Session



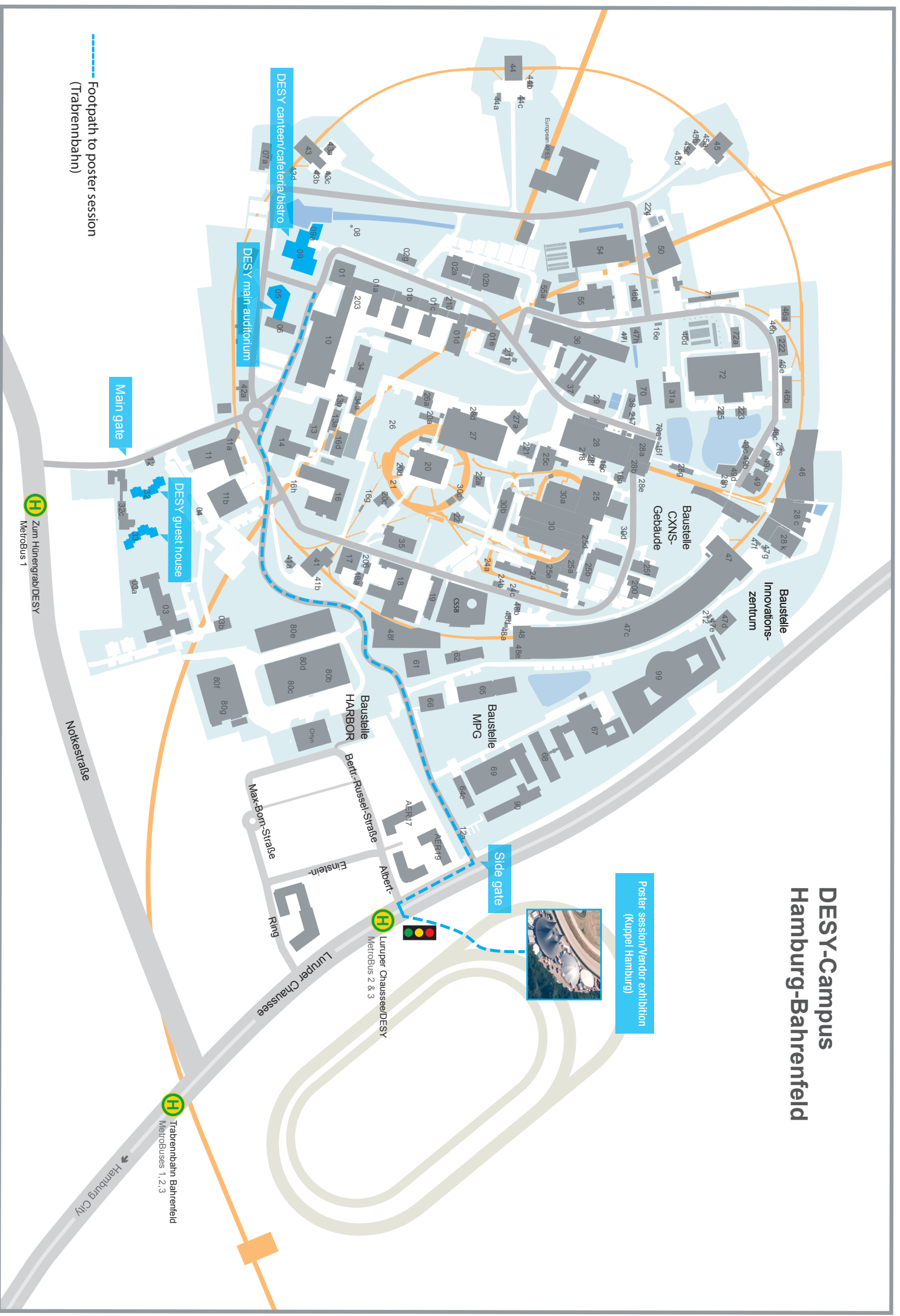
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# DESY-Campus Hamburg-Bahrenfeld



Poster session/Vendor exhibition  
(Kupferkammer)

Side gate

DESY main auditorium

DESY guest house

DESY canteen/cafe/cafeteria/bistro

Main gate

Footpath to poster session  
(Trabrennbahn)

Zum Hünengrab/DESY  
Metrobus 1

Trabrennbahn Bahrenfeld  
Metrobuses 1, 2, 3

Nickseestraße

Max-Born-Station

Lurper Chaussee/DESY  
Metrobus 2 & 3

Hamburg City