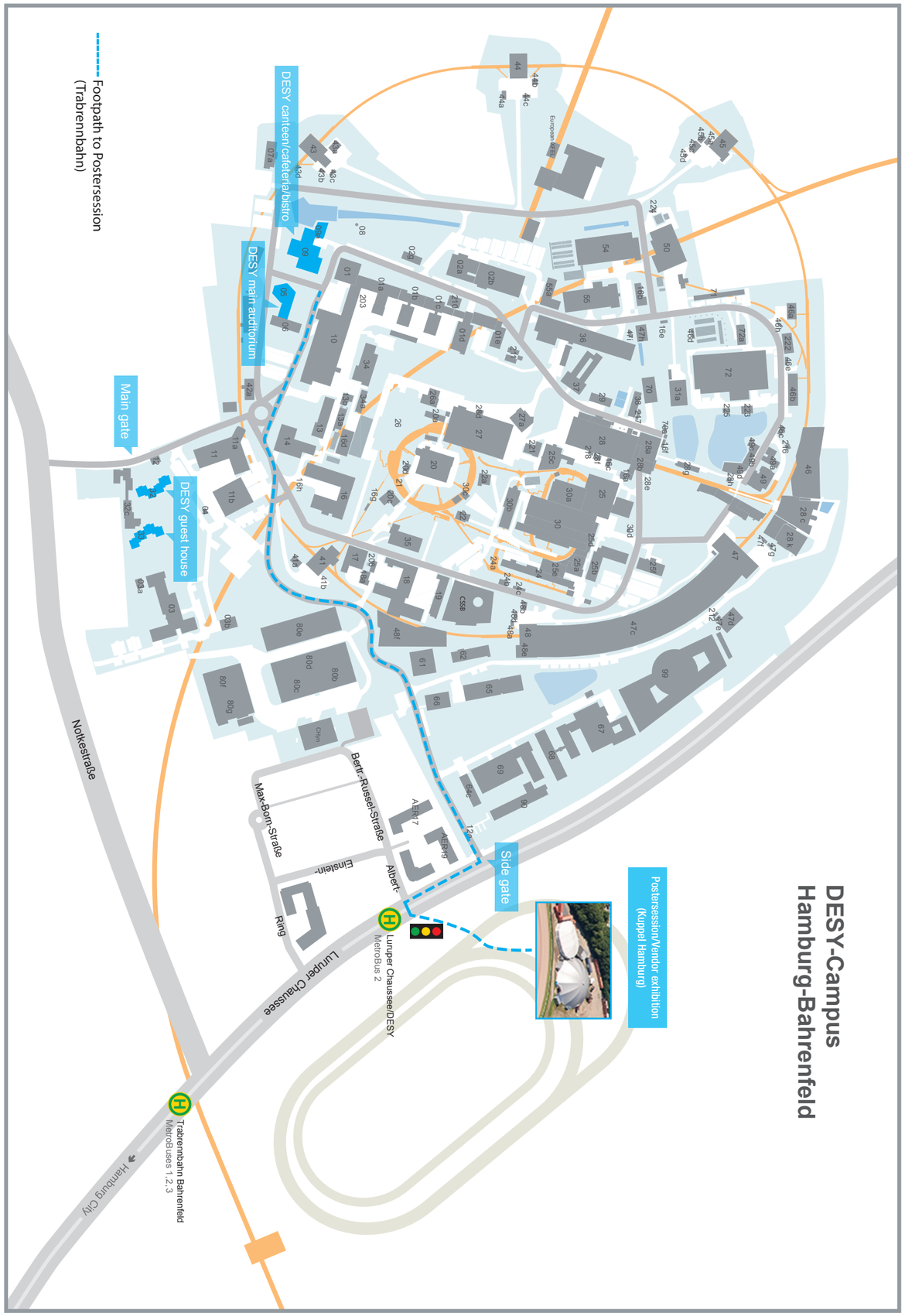

DESY Photon Science Users' Meeting 2018
European XFEL Users' Meeting 2018

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

DESY Photon Science Users' Meeting 2018
European XFEL Users' Meeting 2018

January 2018 in Hamburg

DESY Auditorium (Bldg. 5)

Monday, 22 January: Satellite Workshops

09:15 – 19:00	X-ray diffraction and spectroscopy in very high magnetic fields at the Helmholtz Beamline for Extreme Fields	**European XFEL** | Room E1.173

Tuesday, 23 January: Satellite Workshops

08:30 – 20:00	Early science at the Materials Imaging and Dynamics (MID) instrument	**European XFEL** | Room E1.173
10:00 – 20:00	Early science at High Energy Density (HED) instrument and status of HIBEF contributions	**European XFEL** | Room E1.173
10:00 – 17:00	Data Analysis Workshop and Karabo (CAS)	**DESY** | Bldg. 28c, FLASH Sem. R
09:00 – 12:00	Science using high-energy optical laser systems at High Energy Density beamline - HIBEF	**DESY** | Bldg. 3, Sem. R. BAH 1

Wednesday, 24 January: European XFEL Users' meeting - Plenary Sessions

8:30–10:00	**Registration**		
10:00	Welcome	R. Feidenhans'l	*European XFEL*
10:10	Opening address from the Council Chair	M. M. Nielsen	*DTU, Lyngby*
	Project Update Session	*Chairperson: M. M. Nielsen (DTU)*	
10:20	General status of the project	R. Feidenhans'l	*European XFEL*
10:50	Electron accelerator – commissioning experience and plans	H. Weise	*DESY, Hamburg*
11:20	Photon beamlines commissioning	J. Grünert	*European XFEL*
11:50	SASE3 instruments – status and plans	S. Molodtsov	*European XFEL*
12:20	SASE2 instruments – status and plans	A. Madsen	*European XFEL*
12:50–14:00	**Lunch break**		

Science Session: Early User Experiments and hard X-ray FELs Science Highlights

Chairperson: N. Rohringer (CFEL-DESY)

14:00	FXE: instrument and commissioning progress + highlights	Ch. Bressler	*European XFEL*
14:20	SPB/SFX: instrument and commissioning progress + highlights	A. Mancuso	*European XFEL*
14:40	Revealing the nanoscale structure of viruses with XFEL pulses	R. Kurta	*European XFEL*
15:10	Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions	D. Kraus	*HZDR, Dresden*
15:40-16:10	**Coffee break**		
16:10	Femtosecond response of polyatomic molecules to ultra-intense hard X-rays	B. Erk	*DESY, Hamburg*
16:40	Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers	F. D. Fuller	*LBNL, Berkeley SLAC, Stanford*
17:10	Light-induced ultrafast structural reorganizations in the hybrid perovskites	A. Lindenberg	*Stanford Univ. and PULSE*
18:30	**European XFEL Dinner Reception**	**(in the DESY canteen, Bldg. 9)**	

Thursday, 25 January: DESY Photon Science Users' Meeting - FLASH

8:30–9:00	**Registration**		
			Chairperson: R. Treusch (DESY)
09:00	Welcome	E. Weckert	*DESY, Hamburg*
09:05	FLASH - today and tomorrow - status report and future plans	E. Plönjes-Palm	*DESY, Hamburg*
09:35	Novel FEL lasing schemes with variable gap undulators	E. Schneidmiller	*DESY, Hamburg*
10:00	Concept for a time-compensating monochromator at FLASH2	L. Poletto	*CNR-IFN, Padua*
10:25 - 11:00	**Coffee break**		

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

			Chairperson: S. Molodtsov (European XFEL)
11:00	Magnetic switching in granular FePt layers promoted by near-field laser enhancement	E. Jal	*UPMC Paris*
11:30	Quantum imaging with incoherently scattered light from a Free-Electron Laser	J. von Zanthier	*FAU Erlangen-Nürnberg*
12:00	Coherent diffractive imaging of single helium nanodroplets with a high harmonic generation source	D. Rupp	*Max-Born Institute Berlin*
12:30	New routes to imaging the classical and quantum dynamics of finite systems	T. Fennel	*Univ. Rostock*
13:00	ESUO report	U. Pietsch, *ESUO Chair*	*Univ. Siegen*
13.10 - 14.00	**Lunch break**		

Satellite workshops

14:00–17:45	Light-Matter Interaction: Recent Advances in Theory	**DESY** | Bldg. 99, CFEL Sem. R. II
13:30–18:15	8th Workshop on X-Ray Nanoimaging of Biological and Chemical Systems at PETRA III	**DESY** | Bld. 5 DESY Auditorium
13:40–19:00	Russian-German in-situ and nano-diffraction beamline 12:00 Visit PETRA III beamline P23 (Bldg. 48f, 'Ada Yonath' hall)	**DESY** | Bldg. 99, CFEL Sem. R. I
14:00–19:00	Pump probe laser at FLASH2: status, upgrades, future options	**DESY** | Bldg. 28c, FLASH Sem. R.
14:00–19:30	Extreme Conditions Research at DESY	**DESY** | Bldg. 3, Sem. R. BAH 1
14:00–18:40	X-ray absorption spectroscopy at P64/65	**DESY** | Bldg. 25f, Sem. R. 109
13:00–18:20	SAXS/WAXS/GISAXS User Workshop @ DESY	**DESY** | Bldg. 15, CSSB lecture hall
14:00–18:00	High Performance Online-Data-Analysis (aka fast-feedback) infrastructure, services and software for upcoming photon-science experiments - requirements, plans and proposed	**DESY** | Bldg.1b, Sem. R. 4b
14:00–18:00	High energy X-ray diffraction for Physics and Chemistry	**DESY** | Bldg. 25f, Sem. R. 456
14:00–18:00	Helmholtz-Zentrum Geesthacht GEMS Outstation: Materials Research and High Resolution Imaging	**DESY** | Bldg. 66, Sem. R.
14:00–18:00	Photon Science for Industry: Industrial access and best practice use cases (on invitation)	**DESY** | Bldg. 1b, Sem. R. 4a

19:00 **DESY Reception for speakers and participants** **(in the DESY canteen, Bldg. 9)**

Friday, January 26: DESY Photon Science Users' Meeting

8:30 – 9:00	**Registration**		
			Chairperson: G. Grübel (DESY)
09:00	Welcome	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: M. Schnell (DESY/Univ. Kiel)
10:50	Diffusive dynamics during the high-to-low density transition in amorphous ice	F. Perakis	*Stockholm University*
11:20	Field-free deterministic ultrafast creation of magnetic skyrmions by spin - orbit torques	B. Pfau	*MBI Berlin*
11:50	Flow-assisted assembly of nanostructured protein microfibers	C. Lendel	*KTH Stockholm*
12:20	Protein crystallography in living cells	L. Redecke	*University Lübeck/DESY*
12:50	Report of the User Committee (DPS-UC)	P. Müller-Buschbaum,	*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)

(jointly organised by DESY and European XFEL)

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. Address: Luruper Chaussee 30, 22761 Hamburg.

Vendor exhibition

The vendor exhibition will take place in the in the “Kuppel Hamburg” during the poster session.

Social events and site visit

The European XFEL reception will take place on Wednesday, 24 January, at 18:30 in the DESY canteen (Bldg. 9).

The DESY Photon Science reception will take place on Thursday, 25 January, at 19:00 in the DESY canteen (Bldg. 9).

Visit of the European XFEL site in Schenefeld on 25 January (Thursday afternoon) 🚌
Registration is possible on-site at a display in the foyer of the DESY Auditorium on first come first serve basis (max. 100 people). Departure times of the bus tours are 14:30 and 16:00 on Thursday. They start in front of the DESY Auditorium (Bldg. 5), the visit lasts approx. 2 hours (incl. transfer).

DESY WLAN

Name: UserMeeting2018
WPA/WPA2-PSK: iu4ohcohXuHe

Organizers

S. Bertini (European XFEL), N. Agarwal (European XFEL), P. Grychtol (European XFEL), K. Ivicic (European XFEL), M. Kreuzeder (DESY), W. Laasch (DESY), F. Lehmkühler (DESY), A. Rothkirch (DESY), A. Schwarz (European XFEL), 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.

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

From the DESY main gate walk straight down the street “Zum Hünengrab” (700 – 800m). You will find a bakery, drugstore and other shops as well as restaurants in the vicinity.

I Main sessions
Abstracts of the talks

Revealing the nanoscale structure of viruses with XFEL pulses

Ruslan P. Kurta[1], Jeffrey J. Donatelli[2], Chun Hong Yoon[3], Andrew Aquila[3], Peter H. Zwart[2], Adrian P. Mancuso[1] and the SPI collaboration

[1] *European XFEL, Schenefeld, Germany*
[2] *Lawrence Berkeley National Laboratory, Berkeley, USA*
[3] *Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, USA*

Serial femtosecond crystallography (SFX) at x-ray free electron lasers (XFELs) offers outstanding possibilities for structure determination of complex biological macromolecules which can form crystals. For those structures which cannot be easily crystallized an alternative technique of single particle coherent diffraction imaging (SPI) has been proposed. It was predicted that diffraction patterns from single particles, for instance macromolecules or viruses, can be measured in “destruction before diffraction” experiments at XFELs before the sample is destroyed by intense radiation, and hence their damage-free structure identified. Substantial technical and algorithmic achievements have now made it possible to perform such measurements. However, the limited resolution of the reconstructed biological samples demonstrated so far demands further theoretical and experimental efforts to establish SPI techniques at XFELs [1]. Therefore, alternative methods for structural characterization of nanoscale objects at XFELs are of great interest.

Here we apply the fluctuation x-ray scattering (FXS) technique, which is based on the analysis of x-ray intensity angular cross-correlation functions [2]. We use extremely bright and ultrashort pulses from an XFEL to measure correlations in x-rays scattered from individual biological particles. This allows us to go beyond the traditional crystallography and single-particle imaging approaches for structure investigations. We employ FXS to recover the three-dimensional (3D) structure of aerosolized virus particles from x-ray diffraction data measured with the Linac Coherent Light Source (LCLS) [3, 4]. We determine 2D correlation maps, which comprise a complex fingerprint of the whole 3D structure of a virus (Fig. 1). Our results of model-based structure analysis and ab-initio structure recovery reveal deviations of the virus structures from the expected icosahedral shape [4]. Our findings demonstrate substantial potential of FXS for the future studies of structure and dynamics of biological materials with an XFEL.

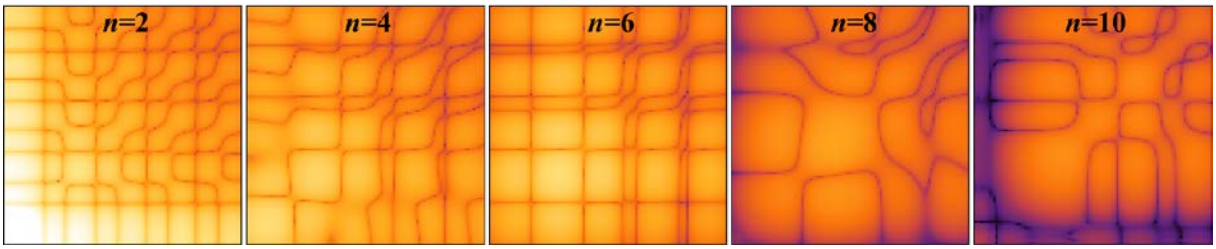

Fig. 1: 2D correlation maps showing the amplitudes of the Fourier components of the orders n=2,4,6,8 and 10 of the angular cross-correlation functions determined for a model of an icosahedral virus.

[1] A. Aquila *et al*., Structural Dynamics **2**, 041701 (2015).
[2] R. P. Kurta, M. Altarelli and I. A. Vartanyants, Adv. Chem. Phys. **116**, 1-39 (2016).
[3] J. J. Donatelli, P. H. Zwart and J. A. Sethian, Proc. Nat. Acad. Sci. **112**, 10286 (2015).
[4] R. P. Kurta *et al*., Phys. Rev. Lett. **119**, 158102 (2017).

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Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions

Dominik Kraus[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf*

High-energy laser systems can be used to mimic extreme states of matter, as found in the interior of various celestial bodies, in the laboratory. Combining such laser systems with extremely bright X-ray sources, particularly X-ray free electron lasers (XFELs), allows for studying exotic physical processes in real-time. This includes high-pressure phase separation reactions, such as diamond precipitation from liquid hydrocarbons, which has been predicted to happen deep inside Neptune and Uranus, and many other interesting phenomena.

At the Linac Coherent Light Source (LCLS), we obtained experimental results from hydrocarbon samples that were laser-compressed to the extreme pressure and temperature conditions found in the deep interiors of such 'icy' giant planets [1]. The extreme brightness of the XFEL source enables unprecedented *in situ* snapshots of the induced chemical reactions and shows that diamond nucleation is initiated on sub-nanosecond timescales at ~150 GPa and ~5000 K. Combining several X-ray and optical diagnostic methods, we obtain high-quality constraints for theoretical models of the involved physical processes: X-ray diffraction records the formation of solid diamond structures, Small angle X-ray scattering determines the size distribution of the growing nanodiamonds while spectrally resolved X-ray scattering provides an absolute scale for the diffraction pattern giving the absolute amount of the reacting material that undergoes species separation. Optical velocimetry is used to characterize and optimize the laser-driven compression waves and optical reflectometry indicates that the isolated hydrogen produced by the phase separation reaction is in a metallic state. All these diagnostics can be used with single-shot quality in the same experiment and provide unprecedented insights into the nanosecond kinetics of chemical reactions at extreme pressures and temperatures.

Besides underlining the general importance of chemical processes inside giant planets, our results will inform mass-radius relationships of carbon-bearing exoplanets, provide constraints for their internal layer structure and improve evolutionary models of Uranus and Neptune, where carbon-hydrogen separation could significantly influence the convective heat transport. Finally, our experiments may identify a new method to produce diamond nanoparticles for material science and industrial applications.

[1] D. Kraus et al., Nature Astronomy 1, 606-611 (2017)

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Femtosecond response of polyatomic molecules to ultra-intense hard X-rays

Benjamin Erk[1]

[1] *Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany*

Today's X-ray Free-Electron Lasers (XFELs) give access to a new extreme regime of light-matter interactions and provide unique, new, capabilities for investigating the structure and dynamics of biological systems, complex materials, and matter under extreme conditions. In particular, this includes serial femtosecond nanocrystallography [1] and the possibility of single-shot imaging isolated non-crystalline particles [2,3]. Many of these applications operate, in the domain of hard X-rays using extremely high peak intensities (exceeding 10^{20} W/cm^2) [2].
However, most experiments investigating smaller atomic and molecular systems with XFELs by looking into the individual response of small constituents of matter have been performed using soft X-rays and much lower intensities.
In a recent study, we investigate how atoms and small polyatomic molecules respond to hard X-ray pulses at intensities approaching 10^{20} W/cm^2 [4]. Our experimental data together with a newly developed theoretical modelling toolkit, demonstrates that under these conditions, the ionization of a molecule is considerably enhanced compared to the case of an individual heavy atom with the same absorption cross section. This finding is qualitatively different from earlier observations in the soft X-ray domain at lower intensities [5,6] or with less intense hard X-ray pulses [7,8]. This enhancement is driven by ultrafast charge transfer within the molecule, which refills the core-holes created in the heavy atom, promoting further inner-shell ionization and resulting in the emission of more than 50 electrons in a single XFEL pulse.

[1] H.N. Chapman et al. Nature 470, 73 (2011).
[2] R. Neutze et al., Nature 406, 752 (2000).
[3] M.M. Seibert et al., Nature 470, 78–81 (2011).
[4] A. Rudenko et al., Nature 545, 129 (2017).
[5] B. Erk et al., Phys. Rev. Lett. 110, 053003 (2013).
[6] B. Erk et al., Science 345, 288 (2014).
[7] K. Motomura et al., J. Phys. Chem. Lett. 6, 2944 (2015).
[8] K. Nagaya et al., Phys. Rev. X 6, 021035 (2016).

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Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers

Franklin Fuller[1,3], Sheraz Gul[1], Ruchira Chatterjee[1], Allen Orville[2], Jan Kern[1], Vittal Yachandra[1], Junko Yano[1]

[1] *Lawrence Berkeley National Laboratory, USA*
[2] *Diamond Light Source, UK*
[3] *SLAC National Accelerator Laboratory, USA*

Time resolved structural and electronic state studies of biocatalysis has emerged as a compelling use-case for X-ray free electron laser (XFEL) sources in recent years. At an XFEL, X-ray diffraction and spectroscopic data can be collected at room temperature and at relatively high dose per shot, in contrast to cryogenic low-dose measurements synchrotron sources collected more routinely. The ultrafast (<50 fs) pulses produced by the XFEL are what enable damage free data collection, as the pulses produce signal from the sample before the onset of radiation damage caused by picosecond time-scale diffusion of photo-generated radicals. As a result, time resolved interrogation of the radiation sensitive reaction intermediates of catalytic centers have become feasible. Catalytic metal centers of metalloenzymes, which pass through high valent states as a part of their reaction cycle, are particularly sensitive to X-ray photo-reduction.

Reactive intermediates of the Oxygen Evolving Complex (OEC) in Photosystem II (PSII) have been studied at XFEL sources over the past few years. We have shown, for PSII and other metalloenzymes, that collecting a combination of X-ray diffraction (XRD) and X-ray emission spectroscopy (XES) from the same XFEL pulse probes the relationship between protein structure/dynamics and chemical state. Additionally, multimodal detection offers a means to analyze effects of sample variability and transient state preparation *in situ*, which is important for complex reaction initiation schemes like that employed for PSII. Implementing a multimodal detection approach, however, places new demands on the sample delivery instrumentation and sample preparation that need to be accommodated for optimal performance. We present here a robust technique of delivering discrete nano-volumes of sample to the XFEL beam at ambient pressure and temperature using a conveyor belt, which enables variety of protein activation schemes (chemical and photochemical). The setup allowed us to prepare and probe time points between S-states of PSII and initiate chemical activation by dioxygen of Ribonucleotide reductase (RNR). By discretizing the sample, we can probe longer solution path lengths (~200 microns) while maintaining a relatively low sample consumption of 4-30 µL/minute. The longer path length improves the rate of signal accumulation for solution spectra when compared to a liquid jet operated at similar flow rates dramatically. Data on both solutions and crystal suspensions of PSII and RNR was collected at the Linac Coherent Light Source (LCLS). From the solution spectra collected at RT, we show the setup can advance PSII. In RNR we see the signature of an intermediate forming enroute to the generation of a known Fe(IV) as the O_2 exposure time is changed, starting from a reduced and anoxic protein solution.

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Light-induced ultrafast structural reorganizations in the hybrid perovskites

Aaron Lindenberg[1]

[1] *Stanford University and PULSE*

I will describe our recent efforts probing the ultrafast atomic-scale distortions that accompany photon absorption in the hybrid perovskites and first experiments in this respect at the European XFEL and at other sources using x-ray / electron diffraction and x-ray / THz spectroscopic techniques. These measurements show evidence for light-induced large amplitude structural reorganizations that may play a key role in the unique functional properties of these materials.

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FLASH - today and tomorrow - status report and future plans

Elke Plönjes[1] and Wilfried Wurth[1,2] for the FLASH group

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[2] *Dept. of Physics, Univ. of Hamburg, Luruper Chaussee 149, 22607 Hamburg, Germany and Center for Free Electron Laser Science, DESY, Notkestr. 85, 22607 Hamburg, Germany*

Following the successful start of parallel user operation of FLASH1 and FLASH2 in 2016, in 2017 a number of updates and new features were added to the FLASH user facility. At the same time, the overall FLASH performance during user operation was again very good with an uptime of close to 97%. The new installations and enhanced functionality of, e.g., data acquisition and controls, aim at widening the range of scientific applications at FLASH while easing the performance of an experiment.
A new double pulse scheme has been tested at FLASH1, which in the future can enhance the opportunities in pump-probe techniques, in particular for the THz-soft X-ray pump-probe experimental station BL3.
At the FLASH2 experimental hall, a number of new systems have been installed. The beamline FL24, which provides an open port for user supplied experiments, has recently been equipped with a Kirkpatrick-Baez (KB) focusing optics with bendable mirrors which allows adapting focus size and position to the users' demands. At beamline FL26, the reaction microscope REMI from the MPIK Heidelberg is installed for advanced AMO (Atomic, Molecular and Optical) physics and molecular femtochemistry experiments. For time resolved experiments, REMI has been recently complemented by a grazing incidence split-and-delay unit (SDU) for soft X-ray pump soft X-ray probe experiments which can now fully profit from the fast wavelength tunability of FLASH2.
A new type of high repetition rate laser based on OPCPA (optical parametric chirped pulse amplifier) technology has proven operation according to its initial performance specifications and was moved into the laser hutch in the FLASH2 experimental hall in 2017. The system will be available for users in the second half of 2018. The talk will review the status of FLASH, present the new instrumental developments and some selected recent achievements.

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View into FLASH2 experimental hall

Novel FEL lasing schemes with variable gap undulators

Evgeny Schneidmiller, Bart Faatz, Marion Kuhlmann, Juliane Rönsch-Schulenburg, Sigfried Schreiber, Markus Tischer, Mikhail Yurkov

DESY, Notkestrasse 85, 22607 Hamburg, Germany

We discuss principles and experimental verification of advanced schemes for X-ray FELs using variable gap undulators (harmonic lasing self-seeded FEL, reverse tape etc.). Harmonic lasing in XFELs is an opportunity to extend operating range of existing and planned X-ray FEL user facilities. Contrary to nonlinear harmonic generation, harmonic lasing can provide much more intense, stable, and narrow-band FEL beam which is easier to handle due to the suppressed fundamental. Another interesting application of harmonic lasing is Harmonic Lasing Self-Seeded (HLSS) FEL that allows to improve longitudinal coherence and spectral power of a SASE FEL. Recently this concept was successfully tested at FLASH2 in the wavelength range between 4.5 nm and 15 nm. That was also the first experimental demonstration of harmonic lasing in a high-gain FEL and at a short wavelength (before it worked only in infrared FEL oscillators). Another interesting scheme that was tested at FLASH2 is the reverse tapering that can be used to produce circularly polarized radiation from a dedicated afterburner with strongly suppressed linearly polarized radiation from the main undulator. Reverse tapering can also be used to produce background-free harmonics in the afterburner. An application of frequency doubling that allowed to reach the shortest wavelength at FLASH is discussed as well.

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Concept for a time-compensating monochromator at FLASH2

Luca Poletto[1], Fabio Frassetto[1], Günter Brenner[2], Marion Kuhlmann[2] and Elke Plönjes[2]

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[2] *Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22603, Germany*

The presentation is focused on the monochromatization of FEL pulses using grating monochromators to go beyond the intrinsic resolution of self-amplified spontaneous emission (SASE) FELs.
The use of gratings to realize XUV monochromators with ultrafast time response is well established for high-order laser harmonics, where the problem of pulse length preservation has been extensively studied (Poletto et al, J. Sel. Top. Quant. Electron. 18, 2012). Both the single- and the double-grating design are used. In the first case, when using a single grating, a residual pulse-front tilt due to diffraction has to be accepted at the output of the monochromator, that can however be minimized by choosing a suitable geometry to obtain temporal responses in the range of few tens of femtoseconds in the XUV (Frassetto et al, Opt. Express 19, 19169, 2011). In the second case, two consecutive gratings are employed: the first one performs the spectral selection on an intermediate slit while the second one corrects for the pulse-front tilt introduced by the diffraction. Double-grating instruments have been already demonstrated to give time resolution below 10 fs in the XUV (Poletto et al, Rev. Sci. Instrum. 80, 123109, 2009; Igarashi et al, Opt. Express 20, 3725, 2012).
In this paper, we present the preliminary design of a monochromator beamline for FLASH2 at DESY. The monochromator is designed for the 50-1000 eV energy range with resolving power higher than 1000 and temporal response below 50 fs over the whole energy range, i.e. a temporal elongation of the initial FEL pulse of below 50 fs. The optical design here discussed originates from the variable-line-spaced (VLS) grating monochromator that is already used at LCLS (Heimann et al, Rev. Sci. Inst. 82, 093104, 2011).
Different from the conditions at LCLS, where the energy range of the monochromator is 500-2000 eV and the pulse front-tilt given by the grating is below 30 fs, FLASH2 is operated at lower energies and thus the stretching given by the single-grating configuration would be unacceptable, as discussed later. Therefore, a second grating is added to realize a time-delay-compensating configuration that corrects for the pulse-front tilt to below 10 fs.
The presentation is organized as follows: the single-grating configuration is initially discussed to show the limitations on the temporal duration of the output monochromatic pulse; then the double-grating configuration is presented and its performances are discussed in detail.

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Magnetic Switching in Granular FePt Layers Promoted by Near-Field Laser Enhancement

Emmanuelle Jal[1,*], Patrick, W Granitzka[1,2], Loïc Le Guyader[1,3], Matteo Savoini[4], Georgi L. Dakovski[5], William F. Schlotter[5], Sebastian Carron[5], Matthias C. Hoffman[5], Olav Hellwig[6], Virat Mehta[6], Yukiko K. Takahashi[7], Jian Wang[7], Alexander H. Reid[1], and Hermann A. Dürr[1]

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Future magnetic data storage media will require magnetic nanoparticles with stable ferromagnetic order at diameters of only 10 nm and smaller. In this respect, granular thin films of the $L1_0$-ordered phase of FePt displaying perpendicular magnetic anisotropy are one of the most suitable storage media, in particular for the heat-assisted magnetic recording technique [1]. To date, the influence of the collective dielectric response of FePt nanoparticles on the magnetization switching has not been studied in detail and the question: *Do the dielectric properties of granular FePt layers affect the laser-assisted magnetic switching of these materials?* remains unanswered. To address this question, we study the well-established ultrafast demagnetization of FePt nanoparticles after a femtosecond (fs) optical excitation [2] to disentangle the spatially varying response of individual nanoparticles. Contrary to the heat-assisted magnetic recording process, any heating effects introduced by the fs excitation here do not heat up the FePt nanoparticles above their Curie temperature [2]. To follow the magnetism dynamics of granular thin FePt films in an out-of-plane applied magnetic field, we performed time-resolved small-angle x-ray scattering experiments with the Soft X-ray Materials Science (SXR) instrument of the Linac Coherent Light Source (LCLS) x-ray free-electron laser at the SLAC National Accelerator Laboratory. We used 1.5 eV ultrashort laser pulses as a pump, and ultrashort soft x-rays pulses in resonance with the *2p – 3d* core-valence L_3 absorption edge of Fe as a probe (Fig. 1).

The analysis of this experiment [3] shows that there is a reproducible switching of a large fraction of the illuminated FePt nanoparticles (red) due to the near-field modifications of the incident laser pulses by neighboring nanoparticles. We quantify the amount of not-switching FePt nanoparticles (black) and demonstrate that the switching probability is enhanced by an increased latency of the deposited laser-energy before being transported to a heat sink [3]. We note that our results are of importance for a microscopic understanding of the recently observed so-called all-optical magnetic switching in FePt granular films.

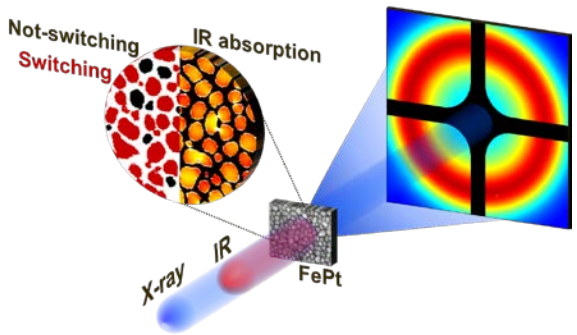

Figure 1. Schematic of a time-resolved small angle x-ray scattering experiments on a FePt granular thin films. The diffraction picture is a true one. The right part of the zoomed picture shows the simulation, from a TEM image, of the infrared absorption by the FePt nanoparticles. The left part represents FePt granular film TEM image color coded according to switching (red) and not-switching (black) nanoparticles.

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Quantum imaging with incoherently scattered light from a Free-Electron Laser

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For more than 100 years, X-rays have been employed in crystallography to determine the structure of crystals and molecules by use of coherent diffractive methods. With the advent of accelerator-driven free-electron lasers (FEL) new avenues for high-resolution structure determination have been explored that go even far beyond conventional X-ray crystallography [1-3]. Yet, these techniques rely on coherent scattering, i.e., processes that maintain the first-order coherence of the radiation field throughout the imaging procedure. For these approaches, incoherently scattered radiation due to, e.g., wave front distortions or fluorescence emission - often the predominant scattering mechanisms -, is considered a detrimental effect. Here we show that schemes from quantum imaging, i.e., exploiting higher order intensity correlations as known from Hanbury-Brown-Twiss interferometry, can be fruitfully applied to image the full 1D, 2D and even 3D arrangement of sources that scatter incoherent X-ray radiation [4-8]. We discuss a number of properties of the method that are conceptually superior to those of conventional coherent X-ray structure determination, We also point out that current FELs are ideally suited for the implementation of the approach [7]. We finally present a recent experimental demonstration in the soft X-ray domain, where we used higher-order intensity correlations to achieve higher fidelities in the image reconstruction and potentially a sub-Abbe resolution [8].

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Coherent diffractive imaging of single helium nanodroplets with a high harmonic generation source

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Highly intense, short XUV and x-ray pulses allow to measure diffraction images of single nanoscale objects in free flight with a single irradiation. From these patterns, formed by the interference of elastically scattered photons, the nanoparticle's structure can be determined. This allows studying non-depositable specimen and short-lived dynamics. Even ultrafast electron dynamics on the nanoscale, such as excitation, ionization and plasma formation in a single particle, change the scattering response and can therefore in principle be followed by diffractive imaging.

Up to recently, single-particle diffraction experiments were only possible at short wavelength free-electron lasers (FELs). A fundamental understanding of the interaction of intense XUV and x-ray pulses with matter was developed, often using atomic clusters as simple, scalable model systems. Also characteristic features of a changing electronic structure could be observed in the diffraction images of clusters, but the changes could not be temporally resolved with the femtosecond FEL pulses. Sub-femtosecond XUV pulses and trains of pulses can however be achieved with high-harmonic generation (HHG) sources based on intense femtosecond lasers, but they are typically orders of magnitude weaker than FELs.

Recently we demonstrated single-particle single-shot diffractive imaging of individual helium nanodroplets using XUV pulses (20 fs, 3×10^{12} W/cm^2) from an extremely intense HHG source. From the bright wide-angle diffraction images, a small fraction of extremely prolate droplets could be uniquely determined, contributing to the current discussion of spinning superfluid droplet shapes. Further, a multicolor Mie approach was developed for the analysis of the patterns consisting of a superposition of several harmonics between 17 and 27 eV. The results of these proof-of-principle experiments, in particular the single-shot extraction of the droplets' complex refractive indices, will build the basis for future time-resolved experiments. By exploiting the exciting characteristics of HHG sources, i.e. jitter-free coherent multicolor pulses and attosecond pulse durations, experiments complementary to FEL research will become possible, aiming at resolving correlated and collective electron motion in highly excited matter on a scale of nanometers and sub-femtoseconds.

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New routes to imaging the classical and quantum dynamics of finite systems

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When compared to atoms and solids, the collective and correlated electron dynamics in finite systems under intense light fields can be substantially modified, enhanced and controlled by plasmonic near-fields [1]. Localized near-fields result from electronic polarization and charge separation, may unfold on femtosecond or even attosecond time scales, and can have various implications on the strong-field physics of nanostructures, nanoparticles, and clusters [2]. Examples include space-charge trapping of photoelectrons [3], waveform-controlled electron acceleration through resonant plasmonic field amplification [4], or directionally controlled surface backscattering [5]. In this talk, two novel routes for characterizing the classical and quantum aspects of the underlying light-matter interactions at the nanoscale will be discussed. Though being fundamentally different conceptually, both schemes have come in reach with current short-wavelength FEL sources providing multicolor pump-probe pulses.

The first scenario – the *"nanoplasma oscilloscope"* – is motivated by previous theory work [6,7] on the XUV ionization of clusters and aims at tracing the complex evolution of space-charge potentials in laser-illuminated nanostructures. Such information is inaccessible with scattering methods such as coherent diffractive imaging but important for the understanding of non-linear plasma formation dynamics, radiation damage and relaxation processes in finite systems. Preliminary experimental data from a recent beam time at FERMI and the related theoretical analysis will be discussed.

The second scenario – the "*quantum coherent diffractive imaging"* (QCDI) - aims at exploring the non-linear response of extended nanosystems through near-field driven bound-state coherent quantum dynamics. A promising route to trace the spatiotemporal population dynamics is the analysis of respective signatures in single-shot diffraction images. We simulated the nonlinear response of Helium droplets under resonant 1s-2p excitation as a model using a coupled quantum-electromagnetic simulation based on a few-level approximation and utilizing the finite-difference time-domain method. The nonlinear modifications of the diffracted field through coherent bound state dynamics will be presented [8]. These illustrate the potential for spatiotemporal characterization of collective excitation dynamics in nanosystems and the development of new metrologies in the emerging field of quantum coherent diffractive imaging.

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Diffusive dynamics during the high-to-low density transition in amorphous ice

Fivos Perakis[1,2], Katrin Amann-Winkel[1], Felix Lehmkühler[3,4], Michael Sprung[3], Daniel Mariedahl[1], Jonas A. Sellberg[5], Harshad Pathak[1], Alexander Späh[1], Filippo Cavalca[1,2], Daniel Schlesinger[1], Alessandro Ricci[3], Avni Jain[3], Bernhard Massani[6], Flora Aubree[6], Chris J. Benmore[7], Thomas Loerting[6], Gerhard Grübel[3,4], Lars G. M. Pettersson[1], and Anders Nilsson[1]

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It has been postulated that the observed high- and low-density amorphous ice forms of water, HDA and LDA, can be related to two hypothesized high- and low-density liquids, HDL and LDL, through two distinct glass transitions in the ultraviscous regime. Here, we study experimentally the structure and dynamics of HDA ice as it is heated up and relaxes into the low-density form. Is this a transition between two amorphous ice forms, i.e., an HDA-to-LDA transition, or is this transition occurring between two liquid states, inferring instead an HDL-to-LDL transition in the ultraviscous regime? The unique aspect of this work is the combination of two X-ray methods, where Wide-Angle X-ray Scattering (WAXS) provides the evidence for the structural changes at the atomic level and X-ray Photon Correlation Spectroscopy (XPCS) in the small-angle X-ray scattering (SAXS) geometry provides insight about the motion at the nanoscale, respectively [1]. The diffusive character of both the high- and low-density forms is discussed among different interpretations and the results are most consistent with the hypothesis of a liquid–liquid transition in the ultraviscous regime.

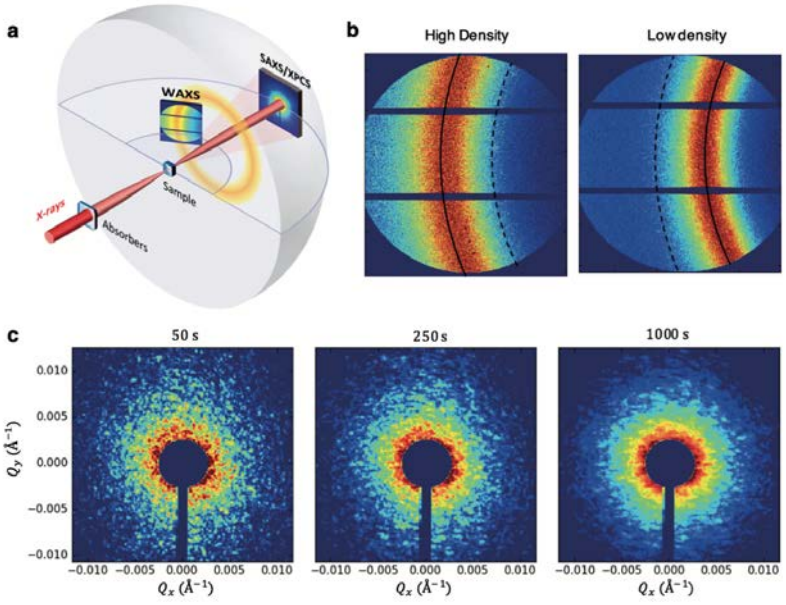

Fig. 1. (a) The experimental setup combining (b) WAXS with (c) XPCS in SAXS.

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Field-free deterministic ultrafast creation of skyrmions by spin–orbit torques

Felix Büttner[1], Ivan Lemesh[1], Michael Schneider[2], Bastian Pfau[2], Christian M. Günther[2,3], Piet Hessing[2], Jan Geilhufe[2], Lucas Caretta[1], Dieter Engel[2], Benjamin Krüger[4], Jens Viefhaus[5], Stefan Eisebitt[2,3], and Geoffrey S. D. Beach[1]

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Skyrmions are chiral spin textures in perpendicular magnetic materials. Their defining property is a spherical topology, which in practical terms means that skyrmions are enclosed by a defect-free closed-loop domain wall. Skyrmions are the smallest non-trivial entities in magnetism and therefore constitute a promising way to encode information in next generation magnetic data storage devices. Generation, transport and annihilation of skyrmions are fundamental operations in this context. Here, we demonstrate that skyrmions can be generated deterministically on subnanosecond timescales in magnetic racetracks using spin–orbit torque pulses. Externally applied in-plane magnetic fields are not required in the process. Skyrmions can be nucleated at natural or artificial structural defects of the magnetic track, allowing one to precisely control the position of the nucleation process. Using micromagnetic simulations, we explain the nucleation process in detail. Our observations provide a simple and reliable means for skyrmion writing that can be readily integrated into racetrack devices.

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Flow-assisted assembly of nanostructured protein microfibers

Ayaka Kamada,[2] Nitesh Mittal,[2,3] L. Daniel Söderberg,[2,3] Tobias Ingverud,[3,4] Wiebke Ohm,[5] Stephan V. Roth,[4,5] Fredrik Lundell[2,3] and Christofer Lendel[1]

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Proteins are Nature's own high-performance materials providing both extraordinary mechanical properties (e.g. muscles, silks) and sophisticated functionality (e.g. adhesion, biological signaling). These materials have served as inspiration for man-made structures for long time but the challenge to produce synthetic materials with comparable properties from biobased resources remains. The key to achieve this is to gain control over the assembly of hierarchical structures from the biomolecular building blocks. Protein nanofibrils have emerged as a promising foundation for the synthesis of novel bio-based materials for a variety of applications. Such nanofibrils are formed through self-assembly and have mechanical properties comparable to silk. Here we demonstrate that micrometer sized protein fibers can be created from protein nanofibrils using a microfluidics setup without the addition of plasticizers or crosslinkers. Microfocus small-angle X-ray scattering allows us to monitor the fibril orientation in the micro channel and compare the assembly processes of nanofibrils of distinct morphologies. The results reveal essential parameters associated with the formation of protein fibers and provide new insights about the assembly processes of hierarchical protein materials.

Reference: Kamada *et al.* (2017) Flow-assisted assembly of nanostructured protein microfibers. *Proc. Natl. Acad. Sci. USA,* 114: 1232–1237.

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Protein crystallography in living cells

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X-ray crystallography requires the growth of well-ordered, sufficiently sized protein crystals to obtain structural insights at atomic resolution. In addition to routinely performed parameter screening *in vitro*, protein crystallization in living cells, referred to as *in cellulo* crystallization, holds the possibility to grow a huge number of micron-sized protein crystals with comparable properties and of high quality in a short time (1-3). The advantage of *in cellulo* crystallization is apparent: The cells grow the protein crystal without the need for purification or crystal screening steps. To systematically exploit the potential of *in cellulo* crystallization in living insect cells for structural biology we streamlined this process by establishing a pipeline to elucidate the structural information of *in cellulo* crystallized target proteins in short time. After cloning of the target gene into baculovirus transfer vectors, the associated recombinant baculoviruses are generated to infect insect cells, and crystal formation is detected at day 4 to 6 after infection. If intracellular crystallization is successful, diffraction data of the isolated *in cellulo* crystals are collected using serial crystallography approaches at XFELs (4) or highly brilliant synchrotron sources (5), depending on the size of the obtained crystals. In our hands, these efforts resulted in the successful crystallization of more than 20 different proteins in living insect cells so far. However, two major bottlenecks currently restrict a more broad application: Depending on the recombinant protein, the number of crystal containing cells varies between more than 70 % and less than 1 %, and changes of environmental conditions during cell lysis and crystal purification result in a loss of crystal quality.

To overcome these limitations we recently established techniques for serial diffraction data collection from *in cellulo* grown crystals directly within living cells using synchrotron and XFEL radiation, combined with intracellular labelling of the recombinant target proteins with heavy metals. These innovative approaches avoid crystal purification and transfer of the living, crystal-containing cells, allow direct screening of cell cultures for successful *in cellulo* protein crystallization using the X-ray beam, and will gain access to direct phasing methods. Thus, our current *in cellulo* crystallization pipeline will be further improved to elucidate structures of proteins without prior information, and limitations in data collection due to low intracellular crystallization efficiency will be overcome, supported by additional integration of fluorescence-based cell sorting. Our results pave the way to more efficiently use crystal containing cells as suitable targets for serial diffraction data collection at synchrotrons and XFELs in the future.

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II Programmes Satellite Meetings

HiBEF

SATELLITE WORKSHOP – Photon Science

X-ray diffraction and spectroscopy in very high magnetic fields at the Helmholtz International Beamline for Extreme Fields

Monday, 22 January 2018 — **European XFEL room E.1.173**

The HIBEF consortium plans to contribute pulsed magnets with peak fields of 60 T and different coil geometries to the HED instrument at the European XFEL. This will offer the possibility to perform x-ray diffraction and spectroscopy experiments under the highest magnetic fields available at any x-ray source in the world. The aim of the workshop is to present the planned infrastructure and discuss new scientific opportunities and early user experiments.

Organisers: C. Strohm, M. von Zimmermann , C. Baehtz and T. Herrmannsdörfer
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PROGRAMME

09:15 -10:00	***Coffee, get together, registration***		
	Opening session: Setting the stage	**Chair: S. Molodtsov**	
10:00	Welcome (10 min)	S. Molodtsov	European XFEL
10:10	Keynote: Recent progress in high magnetic field science at SR and XFEL sources (50 min)	H. Nojiri	Tohoku University
11:00	The HED Instrument (20 min)	U. Zastrau	European XFEL
11:20	Opportunities at European XFEL (20 min)	C. Strohm	DESY
11:40	Pulsed high magnetic fields at HIBEF (20 min)	S. Yamamoto	HZDR HLD
12:00 -13:00	***Lunch break, buffet lunch in the XFEL Foyer***		
	Session 1: Diffraction experiments	**Chair: Z. Islam**	
13:00	High temperature superconductors: diffraction (25 min)	S. Gerber	PSI
13:25	LNCMI coils at radiation sources (20 min)	O. Portugall	CNRS LNCMI
13:45	Day 1 experiments at XFEL (20min)	J. Chang	Universität Zürich
	Session 2: Diffraction experiments	**Chair: S. Gerber**	
14:05	Pulsed fields at the APS (25 min)	Z. Islam	APS
14:30	High field Neutron experiments at HZB (20 min)	O. Prokhnenko	HZB
14:50	Day 1 experiments at XFEL (20 min)	J. Geck	TU Dresden
15:10 -16:10	***Coffee break in the XFEL Foyer***		
	Session 3: Spectroscopy and coherent methods	**Chair: O. Portugall**	
16:10	XMCD experiments with the ESRF miniature coils (20 min)	S. Pascarelli	ESRF
16:30	High temperature superconductors: XAS (20 min)	W. Tabis	TU Wien
16:50	Coherent methods (20 min)	C. Gutt	Universität Siegen
17:10	**Round table: early user experiments.**	**Chair: Organisers**	
	Session 4: MegaGauss and beyond - brainstorming	**Chair: H. Nojiri**	
17:45	Single turn coils (20 min)	O. Portugall	CNRS LNCMI
18:05	Plasma experiments in pulsed fields (20 min)	A. Pelka	HZDR
18:25	Laser driven field generation (20 min)	T. Toncian	HZDR
18:45	***Closing remarks***		

European XFEL Users' Meeting — Satellite meeting:

Early science at the Materials Imaging and Dynamics (MID) instrument

Tuesday, 23 January 2018 - Seminar Room E1.173
Headquarters, European XFEL, Holzkoppel 4, 22869 Schenefeld

The aim of the workshop is to inform about how to apply for beam time at the MID station of the European XFEL and which equipment and operation parameters will be available for the start-up. Possibilities for early science will be discussed by invited speakers and staff. A visit of the experiment hall is possible in connection with the workshop.

Organiser: Anders Madsen

Contact: anders.madsen@xfel.eu

Tuesday, 23 January 2018			
8:00	**Registration starts**		
8:30	**Welcome**	S. Molodtsov	European XFEL
8:45	Introduction to MID	A. Madsen	European XFEL
9:30	Microscopic cryogenic liquid jets as novel tool to study non-equilibrium phase transition at European XFEL	A. Schottelius	University of Frankfurt
10:00	High-Purity X-ray Polarimetry - A Unique Method at MID	K. S. Schulze	University of Jena
10:30	Hard X-ray split-delay line for the MID station	S. Eisebitt	MBI Berlin
11:00	**Coffee**		
11:20	Equilibrium dynamics of deeply supercooled water probed by ultrafast X-ray Speckle Visibility	F. Perakis	Stockholm University
11:50	X-ray diffuse scattering as a probe of anharmonic phonon-phonon coupling in solids	M. Trigo	Stanford University
12:20	Studies of IR laser induced periodic plasma in colloidal crystals probed by XFEL radiation	S. Lazarev	DESY Hamburg
12:50	**Summary & Wrap-up**		
13:00-14:00	**Lunch** (jointly with participants of the MID and HED satellite)		
14:00-18:30	**Proposal discussions and facility tour**		
18:30	**Buffet dinner**		

European XFEL Users' Meeting — Satellite meeting:

Early science at the High Energy Density instrument and status of the HIBEF contributions

Tuesday, 23 January 2018 – Seminar Room E1.173
Headquarters, European XFEL, Holzkoppel 4, 22869 Schenefeld

The aim of the workshop is to inform about how to apply for beam time at the HED instrument of the European XFEL and which equipment and operation parameters will be available for the start-up. Possibilities for early science will be discussed by XFEL staff and members of the HIBEF UC. A visit of the experimental hall is possible prior to the workshop.

Organiser: Ulf Zastrau

Contact: ulf.zastrau@xfel.eu

Tuesday, 23 January 2018			
10:00–12:00	**Start of registration** **Guided tours of experimental hall and the HED instrument** (the MID satellite workshop takes place in E1.173) **Meeting at DESY: Potential kJ laser at the HED instrument**		
12:00–13:20	**Lunch** (jointly with participants of the MID and HED satellite) In the foyer of European XFEL headquarters (XHQ)		
	Early science at the High Energy Density instrument	*Chair:* M. Nakatsutsumi	European XFEL
13:20	Welcome, Overview of HED instrument, Early Science in 2019	U. Zastrau	European XFEL
13:30	X-ray characterization for early science at HED (X-ray properties, harmonic rejection, focusing, monochromators, slits & monitors, timing tool, spectrometer)	Z. Konôpková	European XFEL
13:55	Experimental environment for early science (Interaction chambers; optical lasers, sample stage, x-ray detectors, high- and low resolution x-ray spectrometers)	M. Makita	European XFEL
14:20	Discussion / buffer		
14:30	Status report of BMBF Verbundforschung project: Split-and-Delay Line	S. Roling	WWU Münster
14:45	Status report of BMBF Verbundforschung project: Time resolved micro-diffraction of SHS reactions	B. Winkler	U Frankfurt/M.
15:00	Life as an European XFEL user (UPEX, proposal deadlines, PRP, funding, allocation periods)	S. Bertini	European XFEL User's office
15:30	Discussion / buffer		
15:45	**Coffee break (foyer)**		
	Status of the HIBEF contributions	*Chair: N.N.*	
16:15	Welcome	T. Cowan	HIBEF
16:25	Status of HIBEF instrumentation	C. Bähtz / T. Toncian	HIBEF
17:10	Phase contrast imaging and focusing schemes	A. Schropp	HIBEF
17:30	HIBEF experiments using x-ray polarimetry	H. P. Schlenvoigt	HIBEF
17:50	Discussion / buffer		
18:30	**Dinner Reception** In the foyer of European XFEL headquarters (XHQ)		
20:00	**HIBEF SAC-TAC meeting** (Scientific and technical advisory committees, closed session)	C. Bähtz T. Toncian	HIBEF

European XFEL Users' Meeting — Satellite meeting:

Karabo and Data Analysis Workshop (CAS)

Tuesday, 23 January 2018 - FLASH Seminar room
Building 28c, DESY, Notkestrasse 85, 22607 Hamburg

The data analysis workshop is split into two parts, which can be attended independently (or both together).
The morning session offers a hands-on workshop introducing the Jupyter Notebook for which we invite participants to bring laptops. No prior knowledge of Jupyter is required, although some basic Python knowledge will be useful.
The afternoon session provides an overview of experiment control, and online and offline data analysis provision at European XFEL in Karabo, and introduces particular tools and aspects in more detail.

Organiser: Hans Fangohr

Contact: hans.fangohr@xfel.eu

Tuesday, 23 January 2018			
10:00	**Welcome - Morning session**	H. Fangohr	European XFEL
10:05	Introduction to Jupyter Notebook – session I	T. Kluyver	Jupyter Developer Team
11:15	**Coffee break**		
11:30	Introduction to Jupyter Notebook – session II		
13:00	**Lunch**		
14:00	**Welcome - Afternoon session**	S. Brockhauser	European XFEL
14:05	Introduction to Karabo	*N.N.*	
14:20	Overview to data analysis infrastructure	H. Fangohr	European XFEL
14:30	Detectors and calibration	S. Hauf	European XFEL
15:15	**Coffee break**		
15:45	Online and Offline data analysis at European XFEL	T Michelat	European XFEL
16:30	Discussion	S. Brockhauser	European XFEL
17:00	Close		

SATELLITE WORKSHOP - Photon Science

Light-Matter Interaction: Recent Advances in Theory

Thursday, 25 January 2018 — Bldg. 99, CFEL seminar room II

The workshop aims at presenting recent advances in theoretical research on light-matter interactions. Six invited experts will report on the research highlights covering a broad spectrum of scientific interests ranging from atomic and molecular physics through condensed matter to warm-dense-matter and plasma research. Outline of future developments will be discussed in connection with recent experimental achievements.

Organizers: B. Ziaja, R. Welsch, R. Santra

PROGRAMME

14:00	**Session 1: Chairman: B. Ziaja**		
14:00	Welcome Address	Robin Santra	DESY & University of Hamburg
14:05	The Electron Gas at Warm Dense Matter Conditions	Michael Bonitz	University of Kiel
14:35	Simulations of Dense Plasmas without Pseudopotentials	Charles E. Starrett	Los Alamos National Laboratory
15:05	Ab-initio- and Large-scale Classical Molecular Dynamics Simulations of Laser Excited Silicon and Antimony Films	Martin Garcia	University of Kassel
15:35-16:05	***Coffee break (30 Min.)***		
16:05	**Session 2: Chairman: R. Welsch**		
16:05	Many-electron theory of attosecond pump-probe spectroscopy	Vitali Averbukh	Imperial College London
16:35	Strong Field Solid State Physics	Thomas Brabec	University of Ottawa
17:05	Ultrafast Ionization and Fragmentation Dynamics of Molecules at High X-ray Intensity	Sang-Kil Son	DESY Hamburg
17:35	Closing Remarks	B. Ziaja	DESY Hamburg & INP Krakow
17:45	***End of the Workshop***		

SATELLITE WORKSHOP - Photon Science

8th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III

Thursday, 25 January 2018 — Bldg. 5, DESY auditorium

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 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

	Session 1: Indroduction and biological nano-imaging		Chair: G. Falkenberg
13:30	Welcome & X-Ray Microscopy Today and at PETRA IV	Christian Schroer	DESY/UHH
14:10	K versus L-line based micro-XRF analysis of lanthanides in Earth and planetary science applications	Laszlo Vincze	Ghent University
14:30	Changes in bone structure due to defects in mineralization-control pathways resolved by XRF/XRD tomography	Hendrik Birkedal	Aarhus University
14:50	Analysis of metal metabolism in plants by micro-XRF and micro-XANES at beamline P06	Hendrik Küpper	Academy of Sciences of the Czech Republic
15:10	Water-window Ptychography at P04	Max Rose	DESY
15:30-16:00	***Coffee break (30 Min.)***		
	Session 2: other nano-imaging applications		Chair: C.G. Schroer
16:00	Nano-imaging at P05	Imke Greving	Helmholtz Zentrum Geesthacht
16:20	In operando X-ray characterization of single nanowire devices	Jesper Wallentin	Lund University
16:40	Diffraction imaging of non-FCC gold in bipyramid shaped microcrystals	Milan Sanyal	Saha Institute of Nuclear Physics, India
17:00	Single catalyst nanoparticle imaging under operation conditions	Manuel Abuin	DESY NanoLab
17:20	Expanding frontiers in catalysis research with X-ray microscopy and tomography	Thomas Sheppard	Karlsruhe Institute of Technology
17:40	Ptychographic X-ray imaging of colloidal crystals	Sergey Lazarev	DESY
18:00	Close-out		
18:15	***End of the workshop***		

SATELLITE WORKSHOP - Photon Science

Russian-German in-situ and nanodiffraction beamline

Thursday, 25 January 2018 CFEL, Bldg. 99, Seminar Room I

The Russian-German Nanodiffraction beamline (P23) is located in the recently built Ada Yonath experimental hall. Its scientific case concentrates on physics and chemistry of systems dominated by low dimensional and confinement effects, materials and processes under non-ambient conditions, in situ / in operando techniques. The available instrumentation pool is aimed for multiscale analysis of nanostructured materials and devices. The beamline will go into the commissioning stage in November 2017 and become partially available for user proposals in the spring call 2018.

In this workshop, we shall present the status of the new Russian-German In-situ and Nanodiffraction beamline, discuss special user requirements and make the plans for further developments.

Organisers: Dmitri Novikov, Raphael Grifone Contact: dmitri.novikov@desy.de

PROGRAMME

12:00-13:00	**Beamline visit: Ada Yonath Hall, building 48f**		
13:40	**Session 1**		
13:40	Welcome	Wolfgang Drube	DESY
14:00	Beamline overview, status and development plans	Dmitri Novikov, Raphael Grifone	DESY
14:40	Pulsed layer deposition for in situ applications at synchrotron and neutron beamlines	Ksenia Maksimova	Immanuel Kant Baltic Federal University
15:00	Opportunities for P23 users at the DESY NanoLab	Thomas Keller	DESY
15:20	In operando surface X-ray scattering studies of electrocatalyst interfaces	Olaf Magnussen	Kiel University
15:40-16:25	***Beamline visit and coffee break (45 Min.)***		
	Session 2		
16:25	Kurchatov Synchrotron Radiation Source and Diffraction limited synchrotron facility project	Alexander Blagov	NRC Kurchatov Institute
16:45	Joint application of spectroscopic and diffraction methods for nanoscale object investigation	Alexander Soldatov	Southern Federal University
17:05	In-situ luminescence analysis: new light on mechanisms of chemical reactions	Huayna Terraschke	Kiel University
17:25-17:40	***Coffee break (15 Min.)***		
	Session 3		
17:40	X-ray scattering investigation in confined liquids	Milena Lippmann	DESY
18:00	In situ monitoring of adsorption-induced phase transitions in flexible Metal-Organic Frameworks	Volodymir Bon	TU Dresden
18:20	General discussion: user requirements and future development plans		
19:00	***End of the workshop***		

SATELLITE WORKSHOP - Photon Science

Pump probe laser at FLASH2: status, upgrades, future options

Thursday, 25 January 2018 — Bldg. 28c, Seminar Room FLASH

In August 2018 the FLASH2 pump probe laser will become available for user experiments at FLASH2. The high repetition rate laser is based on OPCPA (optical parametric chirped pulse amplifier) technology and will be transported with dedicated beamlines to the end of FL24 and FL26. In this workshop we want to discuss the experiments enabled by this laser and which upgrades and modifications would be needed in the future. We want to collect all ideas from the user community to plan the further development of the FLASH2 pump probe laser.

Organizers: Ingmar Hartl & Bastian Manschwetus Contact: Bastian.manschwetus@desy.de

PROGRAMME

14:00	**Session 1**		
14:00	Welcome	B. Manschwetus	DESY
14:10	The FLASH 2 pump probe laser system	T. Lang	DESY
14:40	Design and setup of a permanent HHG beamline at FLASH 2	M. Kovacev	Leibniz Universität Hannover
15:00	IR-FEL pump-probe experiments with the REMI at FLASH 2	R. Moshammer	MPI Heidelberg
15:30-16:00	***Coffee break (30 Min.)***		
	Session 2		
16:00	Spectroscopy to study dynamics in and on solids	M. Beye	DESY
16:30	Tunability in the UV regime allow for novel ultrafast FLASH studies in soft condensed matter	S. Techert	DESY
17:00	Pump pulse considerations for the investigation of magnetization dynamics	J. Lüning	UPMC
17:30-18:00	***Coffee break (30 Min.) / or End of the workshop***		
	Session 3		
18:00	Dynamics in gas-phase biomolecules	S. Bari	DESY
18:15	Contributed talk	N.N.	N.N.
18:30	Contributed talk	N.N.	N.N.
18:45	Discussion and Close-Out	B. Manschwetus	DESY
19:00 (or earlier)	***End of the workshop***		

SATELLITE WORKSHOP - Photon Science

Extreme Conditions Research at DESY

Thursday, 25 January 2018 — **Bldg. 3, seminar room BAH1**

Extreme Conditions Research at high pressure and simultaneous high and low temperatures continues to grow at DESY. Planetary and materials research at low and moderate pressures can be performed at the ECB (P02.2) and at the LVP beamline (P61.2), although at P61.2 without X-rays until beamline construction is complete (projected for end of 2018). Research at extreme pressures (> 60 GPa) can only be performed at P02.2 using the diamond anvil cell (DAC). Furthermore, Extreme Conditions Research is also performed more frequently at other beamlines of PETRA III. New possibilities for research at both cold compressed and WDM will emerge from DESY's contribution to the HIBEF project located at the HED Instrument of the European XFEL. In addition, we have started to develop the Conceptual Design Report (CDR) for Extreme Conditions Research at a diffraction limited storage ring, proposed for PETRA IV in the midterm. Within this satellite meeting we will present ongoing research from different user groups at the different high-pressure beamlines of PETRA III, give a status report on the DAC platform at the European XFEL and give an outlook on the current status of the Extreme Conditions CDR for PETRA IV.

Organisers: R. Farla & H. P. Liermann

Contact: robert.farla@desy.de & hanns-peter.liermann@desy.de

PROGRAMME

14:00	**Session 1: The Extreme Conditions Beamline (115 min.)**	**Chair: R. Farla**	
14:00 – 14:20	Status & Future developments at the ECB beamline at PETRA III	H. P. Liermann	20 min.
14:20 – 14:45	Phase transition in metals at high compression rates in dynamic DAC	Z. Jenei	25 min
14:45 – 15:05	Superfast X-Ray diffraction of $Mg_{0.8}Fe_{0.2}O$ across the spin transition under dynamic compression	A. Mendez	20 min
15:05 – 15:30	Tracking chemical heterogeneities in the Earth's mantle from plasticity studies on minerals under extreme conditions	C. Sanchez Vales	25 min
15:30-16:00	***Coffee break (30 Min.)***		
16:00 – 16:25	*In situ* CO_2 laser heating at an X-ray diffraction beamline	D. Smith	25 min
16:25	**Session 2: The Large Volume Press Beamline (65 min.)**	**Chair: H. P. Liermann**	
16:25 – 16:50	Status of the LVP beamline at PETRA III	R. Farla	25 min.
16:50 – 17:10	High-pressure glass crystallization of transparent nano-ceramics consisting of birefringent crystals with low chromatic aberration	N. Gaida	20 min.
17:10 – 17:30	Fabrication of toughened hard polycrystalline materials and elucidation of the toughening mechanism	E. Kulik	20 min.
17:30-18:00	***Coffee break (30 Min.)***		
18:00	**Session 3: Future Developments for Extreme Conditions Research at DESY (60 min.)**	**Chair: K. Glazyrin**	
18:00 – 18:20	Status of the DAC setup at the HED Instrument of the European XFEL within the framework of the HIBEF Project	H. P. Liermann	20 min.
18:20 – 18:40	Status of the CDR for PETRA IV a DLSR	H. P. Liermann & R. Farla	20 min.
18:40 – 19:00	Discussion about the CDR and Close-Out	R. Farla and H. P. Liermann	20 min.

19:30 (or earlier) ***End of the workshop***

SATELLITE WORKSHOP - Photon Science

X-Ray Absorption Spectroscopy at P64/P65

Thursday, 25 January 2018 **Bldg. 25b, Seminar Room 109**

P64 and P65 -- the new EXAFS-Beamlines in the PETRA III extension – were in full user operation mode in 2017. 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. 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
wolfgang.caliebe@desy.de

PROGRAMME

14:00	**Session 1: (90 Min.)**		
14:00	Status and future plans of P65	E. Welter	(DESY)
14:20	P64: The first year of user operation	V. Murzin .	(DESY)
14:40	QEXAFS at P64	B. Bornmann	(U. Wuppertal)
15:10	Status and preliminary results of the high-resolution XES-spectrometer at P64	A. Kalinko	(U, Paderborn)
15:30-16:00	***Coffee break (30 Min.)***		
	Session 2: (90 Min.)		
16:00	Unravelling structural dynamics in exhaust gas catalysts by *operando* X-ray absorption spectroscopy	A. Gänzler	(KIT)
16:20	Recent examples of chemical research at beamlines P64 and P65	M. Bauer	(U, Paderborn)
16:40	Current status of cell development for *operando* studies at P65	A. Jentys	(TUM)
17:00	Analysis of homogeneous and heterogeneous catalysts employing the SynRAC reactor setup	N. Heidenreich	(CAU Kiel/DESY)
17:30-18:00	***Coffee break (30 Min.) / or End of the workshop***		
	Session 3: (60 Min.)		
18:00	Probing ore formation with a new hydrothermal apparatus at DESY	S. Klemme	(U. Münster)
18:20	Close-out Discussion	E. Welter, W. Caliebe	(DESY)
18:40	***End of the workshop***		

SATELLITE WORKSHOP - Photon Science

SAXS/WAXS/GISAXS-User Workshop @ DESY

Thursday, 25 January 2018 — Bldg. 15, CSSB lecture hall

This workshop addresses current and potential users of small- and wide-angle X-ray scattering at PETRA III. It is intended to present and discuss the status and perspectives of the experimental facilities, especially the PETRA III micro- and nanofocus X-ray scattering beamline P03 (MiNaXS), and recent as well as planned user activities. It shall foster communication among the users and identify common interests.

Organisers: Stephan V. Roth & Rainer Gehrke Contact: Stephan.roth@desy.de

PROGRAMME

13:00	**Session 1: General (15 Min.)**		
13:00-13:15	Welcome & Developments at P03	Stephan V. Roth	DESY & KTH (S)
13:15	**Session 2: Organic photovoltaics (45 Min.)**		
13:15-13:30	Wet-based polymer nanoparticle hybrid materials for electronics	Peng Zhang	INM Saarbrücken
13:30-13:45	Understanding solar cells structure and functioning via GISAXS and GIWAXS	Peter Müller-Buschbaum	TU München
13:45-14:00	An insight into atmospheric degradation processes by mapping local nanoheterogeneities within hybrid polycrystalline perovskite films	Shambhavi Pratab	TU München
14:00	**Session 3: 3D mesoscopic materials (30 min)**		
14:00-14:15	Spatially resolve studies of nanoporous gold speciment at P03 nanofocus endstation	Anton Davydok	HZG
14:15-14:30	Study on conductive silver nanowire networks in 3D printed polymers	Lewis Akinsinde	University of Hamburg
14:30-15:00	***Coffee break (30 Min.)***		
15:00	**Session 4: Surfaces (60 Min.)**		
15:00-15:15	Tracking gyroid self-assembly in polymer films during solvent annealing using in situ GISAXS	Ilja Gunkel	University of Fribourg (CH)
15:15-15:30	Tailoring of uniaxial magnetic anisotropy in Permalloy thin films using nano rippled Si substrates	Sarathlal Koyiloth Vayalil	IIT Bangalore (IND)
15:30-15:45	Structural analysis of size-selected ultrasmall Au clusters using GISAXS	Deniza Chekrygina	University of Hamburg
15:45	**Session 5: Polymer thin films**		
15:45-16:00	In-situ GISAXS studies of solvent vapor annealing of diblock and starblock copolymers	Dorthe Posselt	Roskilde Univ. (DK)
16:00-16:15	Our µ-focus on polymeric thin films	Jochen Gutmann	Univ Duisburg-Essen
16:15-16:45	***Coffee break (30 Min.)***		
16:45	**Session 6: Polymers, composites and fibres (85 Min.)**		
16:45-17:00	Microfluidics and cellulose	Daniel Söderberg	KTH & WWSC(S)
17:00-17:15	Cellulose-PEDOT:PSS spraying	Volker Körstgens	TU München
17:16-17:30	Structure determination during functional stack build-up of power fibres	Sebastian Grott	TU München
17:30-17:45	Real-Time Monitoring of pi-Stacking of Pentacene on Graphene	Peter Siffalovic	SAS (SK)
17:45-18:00	Combination of X-ray-scattering with thermography for advanced investigations of the energy balance during deformation experiments	Konrad Schneider	IPF
18:00-18:15	In-situ time-resolved study of nanoparticles in a plasma source	Jaroslav Kousal	Charles University Prague (CZ)
18:15-18:20	Concluding remarks	Stephan V. Roth	DESY & KTH (S)
18:20	**End of the workshop**		

SATELLITE WORKSHOP - Photon Science

High Performance Online Data Analysis

Thursday, 25 January 2018 — Bldg. 1b, Seminar Room 4b

Looking ahead 3-5 years, we anticipate that both data volumes and data rates from detectors at light source facilities will continue to grow, and that ever more sophisticated experiments by researchers will place correspondingly more intense demands on storage and computing capacity. Experiments employing fast area detectors impose the most severe requirements on the IT infrastructure in terms of network bandwidth, storage capacity and compute power. A move towards on-the-fly processing where possible as a means of handling the data deluge from modern detectors and ever more brilliant light sources, delivering final results (3D volume, ptychographic reconstruction) and not retaining every data frame indefinitely. These, also called near-real-time data analysis, targeted for - rapid experiment feedback, data reduction and many more.

This meeting aimed for bringing together interested people in that topic from various sites, presenting and discussing plans, work-in-progress or currently used solutions

Organisers: T. Kracht, S. Yakubov, M. Gasthuber

Contact: martin.gasthuber@desy.de
thorsten.kracht@desy.de
sergey.yakubov@desy.de

PROGRAMME

14:00	**Session 1**		
14:00	Welcome, Introduction	M. Gasthuber	DESY
14:10	User-Stories		
	20 min	U. Lienert	DESY
	10 min	S. Düsterer	DESY
	20 min	C. Roseman	DESY
	20 min	J. Garrevot	DESY
	10 min	T. Wilksen	DESY
15:30-16:00	***Coffee break (30 Min.)***		
	Session 2		
16:00	Status & Plan of development @DESY/IT (2 presentations)	S. Yakubov	DESY
17:00	WIPs (work in progress) other Labs/Scientists	T.B.D.	
17:15	Wrap-up, Next steps	Organisers	
17:30-18:00	***Coffee break (30 Min.) / End of the workshop***		

SATELLITE WORKSHOP - Photon Science

High Energy X-ray Diffraction for Physics and Chemistry

Thursday, 25 January 2018 — Bldg. 25f, seminar room 456

High energy X-ray diffraction based techniques have a unique impact on physics and chemistry, especially with respect to the formation of materials. This workshop brings together experienced users, interested researchers, and beamline staff to present and discuss the current and future high-energy X-ray diffraction capabilities at DESY and key experiments that demonstrate the potential of this technique.

Organisers: Martin von Zimmermann; Ann-Christin Dippel Contact: martin.v.zimmermann@desy.de
ann-christin.dippel@desy.de

PROGRAMME

14:00	**Session 1**		
14:00	Status Powder Diffraction Beamline P02.1	Michael T. Wharmby	DESY
14:30	Status High Energy X-ray Diffraction Beamline P21.1	Martin von Zimmermann	DESY
15:00	Status High Energy X-ray Diffraction Station P07-DESY	Ann-Christin Dippel	DESY
15:30-16:00	***Coffee break (30 Min.)***		
16:00	**Session 2:**		
16:00	Confining metal-halide perovskites in nanoporous thin films: a high energy WAXS and SAXS study	Bert Nickel,	LMU München (D)
16:30	In-situ / ex-situ Experiments at Synchrotron and Neutron Facilities for Battery Research	Michael Knapp	KIT (D)
17:00	Combining High Energy X-ray Diffraction Techniques with Laser-Induced Fluorescence in Operando Catalysis	Uta Hejral	Lund University
17:30	Discussion		
18:00	***End of the workshop***		

SATELLITE WORKSHOP - Photon Science

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

Thursday, 25 January 2018 — **Seminar Room Bldg. 66**

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 2018 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

			Chair: C. Krywka
	Session 1: Imaging		
14:00	Imaging instruments at IBL, HEMS and MINAXS beamlines	Christina Krywka	HZG, Inst. of Materials Research
14:15	Head Biomechanics of a Springtail	Peter Rühr	Centre for Molecular Biodiversity Research Bonn
14:40	The NOVA project: maximizing beam time efficiency through synergistic analyses of SRµCT data	Philipp Lösel	U Heidelberg, Engineering Mathematics and Computing Lab
15:05	Imaging of bulk supercrystalline nanocomposite materials	Diletta Giuntini / Berta Domenech	TU Hamburg, Inst. of Advanced Ceramics
15:30	***Coffee break 30 min***		
	Session 2: Diffraction		Chair: P. Staron
16:00	Status of the diffraction beamlines	Peter Staron	HZG, Inst. of Materials Research
16:15	Real time monitoring of phase transformations and stress development during rapid surface processing	Jens Gibmeier	KIT, Inst. f. Angewandte Materialien
16:40	Development of advanced β-stabilised titanium aluminides using X-ray diffraction and scattering techniques	Petra Erdely	Montanuniversität Leoben, Departm. of Phys. Metall. and Testing
17:05	*In situ* investigation of friction stir welded steels using high-energy X-ray diffraction	Malte Blankenburg	HZG, Inst. of Materials Research
17:30	***Final discussion***		

III Poster Session

III Poster Session Topics

III.1 Internal/Facility Poster

1. PETRA III at DESY: High Energy Photons at Highest Spectral Brightness
   O.H. Seeck

2. P11 at PETRA III: A Versatile Beamline for Serial and High-Throughput Crystallography
   A. Burkhardt, O. Lorbeer, E. Crosas, S. Günther, T. Pakendorf, B. Reime, J. Meyer, P. Fischer, N. Stübe, M. Warmer and A. Meents

3. The European Cluster of Advanced Laser Light Sources - Status in Final Year
   G.A. Appleby and T. Tschentscher

4. ASAP3 - Current state and services for PETRA III and FLASH
   M. Gasthuber, S. Dietrich, M. Kuhn, U. Ensslin, G. Smirnov, B. Lewendel, J. Malka, C. Patzke, J. Hannapel and S. Yakubov

5. ASAP3 - extensions and new services for next generation experiments at PETRA III and FLASH
   M. Gasthuber, S. Dietrich, M. Kuhn, U. Ensslin, B. Lewendel, J. Malka, C. Patzke, J. Hannapel and S. Yakubov

6. X-Ray Absorption Spectroscopy at P64
   W.A. Caliebe, V. Murzin, M. Görlitz, A. Kalinko and M. Naumova

7. Recent trends in Nuclear Resonant Scattering at P01 PETRA III
   H.-C. Wille, P. Alexeev, O. Leupold, I. Sergeev, R. Steinbrügge, F.-U. Dill and S. Mayer

8. DESY - Insights into matter
   S. Jaehmlich, M. Bierbaum, O. Wendt, L. Fimmen, I. Mahns, S. Moeller, C. Classen and A. Willner

9. X-ray absorption spectroscopy at beamline P65
   E. Welter, M. Herrmann and R. Nemausat

10. The Small-angle X-ray scattering beamline P62 at the PETRA III Extension
    S. Haas and S. Pfeffer

11. FL24 characterization
    T. Wodzinski, B. Keitel, M. Kuhlmann, M. Ruiz-Lopez, S. Künzel and E. Ploenjes-Palm

12. Status of the sidestation P21.1 of the Swedisch Beamline at the PETRA III Extension
    M. v. Zimmermann, R. Nowak, S. Sonntag and O. Gutowski

13. FLASH DAQ and Controls
    M. Degenhardt, S. Düsterer, S. Grunewald, E. Müller, C. Passow and K. Tiedtke

14. DESY NanoLab
    H. Noei, V. Vonk, T. F. Keller and A. Stierle

15. Materials Imaging and Dynamics (MID) Instrument at the European XFEL
    U. Boesenberg, G. Ansaldi, A. Bartmann, K. Chan, J. Hallmann, I. Lobato, W. Lu, J. Möller, M. Reiser, A. Schmidt, M. Scholz, R. Shayduk, A. Zozulya and A. Madsen

16. Status and New Developments at the Extreme Conditions Beamline (ECB, P02.2) at PETRA III
    H. P. Liermann, K. Glazyrin, A. Pakhomova, E. Bykova, M. Bykov, M. Wendt, S. Wenz, A. Ehnes, I. Schwark and J. T. Roehr

17. Maxwell - High Performance Computing for Photon Science
    Y. Kemp, F. Schluenzen, S. Sternberger and S. Yakubov

18. Sample environments and user support at the European XFEL Facility
V. Bazhenov, J. Bielecki, C. Deiter, E. Delmas, K. Dörner, R. Graceffa, Y. Gül M. Kitel, K. Lorenzen, J. Makroczyova, J. Moore, E. Round, R. Schubert, P. Thute and D. Watts

19. Russian-German in-situ and nano-diffraction beamline at PETRA Extension
D.V. Novikov, R. Grifone and J. Raabe

20. The High Resolution Diffraction Beamline P08
F. Bertram, R. Kirchhof, G. Bussone, C. Shen, S. Volkov, O. Gutowski and O. H. Seeck

21. Data processing and storage for European XFEL
N. Al-Qudami, D. Boukhelef, S. Dietrich, U. Ensslin, M. Gasthuber, J. Hannappel, L. Maia, J. Malka, M. Manetti, B. Lewendel, C. Patzke, G. Previtali, J. Szuba, K. Wrona and S. Yakubov

22. European XFEL Data Acquisition System - first experience
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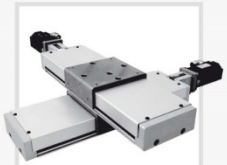

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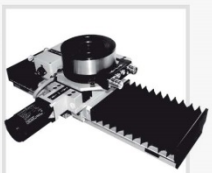

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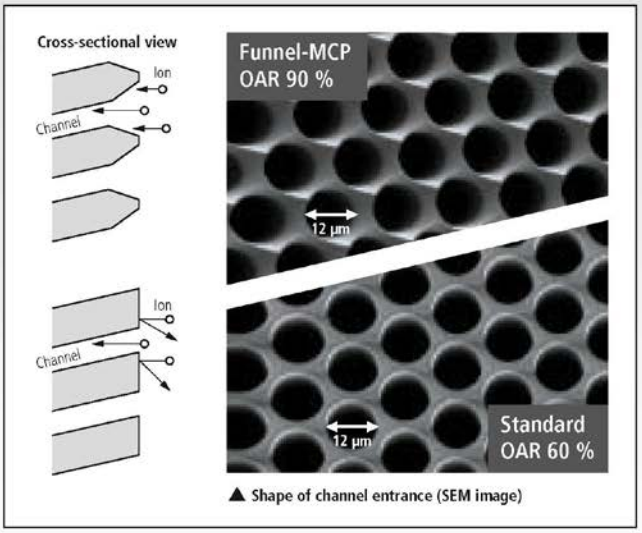
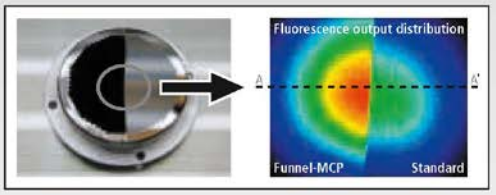
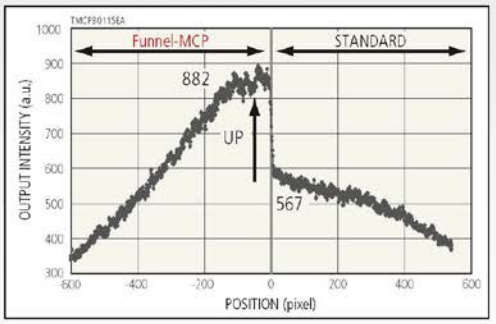


▲ Shape of channel entrance (SEM image)

Example of ion detection



Fluorescence output intensity profile (A-A')



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127. The 4MPix Adaptive Gain Integrating Pixel Detector for the SPB/SFX instrument at the Eu.XFEL
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128. Highly efficient end station for space-, time- and spin-resolved photoemission spectroscopy at free electron lasers.
D. Kutnyakhov, F. Pressacco, G. Mercurio, L. Wenthaus, H. Meyer, S. Gieschen, K. Bühlmann, S. Däster, R. Gort, D. Curcio, K. Volckaert, M. Bianchi, Ch. Sanders, J. Miwa, S. Ulstrup, A. Oelsner, C. Tusche, Y.J. Chen, D. Vasilyev, K. Medjanik, G. Brenner, S. Dziarzhytski, H. Redlin, J. Demsar, H.J. Elmers, Ph. Hofmann, G. Schönhense, Y. Acremann and W. Wurth

129. Towards time-resolved atomic structure determination by means of x-ray standing waves at a FEL
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140. Time-resolved X-Ray diffraction experiments for electric field-induced effects investigation
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145. Near L-edge Single and Multiple Photoionization of Singly Charged Iron Ions
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150. Photoionization and Photofragmentation of $Sc_3N@C_{80}^-$ and $Sc_3N@C_{80}^+$ Ions in the Photon Energy Ranges 17 - 80 eV and 280 - 420 eV
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151. Near-K-edge double and triple detachment of the F^- negative ion: Observation of direct two-electron ejection by a single photon
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155. Anionic Hosts for the Incorporation of Cationic Guests
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157. Ion-source Development for Inner-Shell Photodetachment of Negative Ions
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159. FLASH measurements of the conductivity of warm dense water
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160. Electron behavior in the electrical breakdown
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161. Finite Temperature Opacity and GW Calculations in Aluminium
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163. Structural analysis of size-selected ultrasmall Au clusters using GISAXS
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164. Spin dependent fragmentation dynamic of a core hole excited diradical molecular ion
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165. Time-resolved study of free-free opacity in dense aluminium plasma
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167. Investigation of photo-induced processes within biomolecular systems in the gas phase
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168. The Small Quantum Systems - SQS Instrument at the European XFEL
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169. Time-Resolved Ion- and Electron Spectroscopy of Small Halogenated Molecules
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170. Nuclear resonance scattering of a trinuclear iron complex
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171. A pure molecular beam of water dimer
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172. Effect of X-ray-induced electron ballistic transport on the optical properties in silicon
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173. Low temperature plasmas induced in gases by irradiation with intense EUV pulses
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174. Three-dimensional shapes of spinning superfluid quantum droplets
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177. Non-dipole effects in 3D angular distributions using soft X-rays
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178. Ultra-fast solid to solid phase transition in diamond
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179. Noncollinear spin arrangements in small, size-selected FeV clusters on Cu(100)
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180. Time-dependent atomic physics in the interaction of ultraintense X-ray laser with matter
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181. Laboratory for individual analysis of functional nanoparticles: NP-Facility
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182. Climbing the rotational ladder to chirality
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183. Cryogenically cooled beams of bio-nanoparticles
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184. Soft x-ray spectroscopy of the plasma interface
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185. The photo physics of polycyclic aromatic hydrocarbons studied with FLASH
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186. Toward Imaging Molecular Dynamics through Electron Diffraction and Fragmentation Using a Nanosecond Event Counting Detector
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187. X-ray photophysics and solvent-bond breaking of molecules and clusters
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188. Fragmentation dynamics of methyl iodide upon multiphoton core ionization
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189. Grazing-Incidence XUV Split-Delay Unit for the FLASH2 Reaction Microscope
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190. Reaction Microscope Endstation at FLASH2
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191. COMOTION - Controlling the motion of large molecules and particles
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192. Structural dynamics upon photoexcitation-induced charge transfer in a dicopper(I)-disulfide complex
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193. Molecular-frame strong field ionisation of complex molecules
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194. Nonlinear spectroscopy with chirped x-ray pulses
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195. Photofragmentation of hemin cations in the VUV energy range
K. Schubert, L. Schwob, S. Dörner, T. Schlathölter and S. Bari

196. Inner-shell spectroscopy of simple building blocks of biomolecules
K. Schubert, S. Klumpp, S. Dörner, L. Schwob, S. Deinert, K. Mertens, I. Baev, J. Schunck, M. Kitel, B. Rudek, T. Buhr, A. Müller, S. Schippers, M. Martins and S. Bari

197. Towards site-specific photofragmentation of complex biomolecules.
S. Dörner, K. Schubert, L. Schwob, C. Bomme, R. Boll, S. Deinert, S. Düsterer, D. Egorov, B. Erk, R. Hoekstra, K. Idzik, K. Kubicek, E. Müller, G. Reitsma, D. Rompotis, T. Schlathölter, S. Toleikis, S. Techert and S. Bari

198. Table-top Attosecond Pulses for Nonlinear Spectroscopy in the 100 eV Spectral Region
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200. Phase space based stochastic modeling of amplified spontaneous emission
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201. Simulations of high intensity x-ray induced dynamics of matter
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202. Cultivation time of epidermal cell culture model systems impacts the stratum corneum structural organization: A SAXS investigation
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203. Analyzing protein liquid dense clusters - intermediates in the nucleation process - as potential samples for future XFEL experiments
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204. Revealing the nanoscale structure of viruses with XFEL pulses
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205. Pink-Beam Serial Crystallography
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206. Formation of protein crystal growth units in lysozyme solution studied by small-angle x-ray scattering
K.B. Ilina, A.S. Boikova, Yu.A. Dyakova, P.V. Konarev, A.E. Kryukova, M.A. Marchenkova, A.E. Blagov, Yu.V. Pisarevsky and M.V. Kovalchuk

207. Structural characteristics of CBS-pyrophosphatase from Desulfitobacterium hafniense in solution: SAXS study
L. Dadinova, V. Anashkin and E. Shtykova

208. Octamer formation in lysozyme solutions at the initial crystallization stage detected by small-angle neutron scattering
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209. CrystFEL: Data processing for serial crystallography
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210. Soft x-ray absorption spectroscopy on photosystem II and prototypical manganese complexes in solution
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211. Process of crystallization in starved E. coli cells studied by synchrotron small angle scattering
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212. IL-1 Family Cytokines Use Distinct Molecular Mechanisms to Signal through Their Shared Co-receptor
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213. Insights into the magnetic coupling of iron and heterometals of FeMo and FeV cofactors of Nitrogenase
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214. Table top spectroscopy complements FEL experiments on bio-molecules at the ELI beams facility
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215. Development of biological system for Huntington disease research
C. Rumancev, T.Vöpel, S. Stuhr, A. R. von Gundlach, T. Senkbeil, M, Osterhof, S. Ebbinghaus, T. Saldit, M. Sprung, S. Ebbinghaus and A. Rosenhahn

216. Soft X-ray Fluorescence with STXM Setup - First Results of Biomedical Applications
L. Lühl, K. Andrianov, A. Haidl, H. Dierks, A. Dehlinger, T. Nisius, T. Wilhein and B.Kanngießer

217. Correlated spin and structural dynamics in the recombination of NO to deoxy-Myoglobin in physiological media studied with XES
D. Kinschel, C. Bacellar, F. Alves Lima, B. Sorokin, O. Canelli, G. Mancini, J. Budarz, W. Gewalda, P. Zalden, S. Schulz and M. Chergui

218. Tomography and spectroscopy to study Arsenic and Zinc metal metabolism in plants.
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219. Interaction of NKX2.1 with DNA
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220. P14: Phase contrast X-ray imaging for crystal detection in Lipid Cubic Phase
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221. X-ray speckle visibility spectroscopy using radiation sensitive samples
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222. Serial Synchrotron Crystallography
K.R. Beyerlein, O. Yefanov, M.O. Wiedorn, J. Knoska, A. Tolstikova, E. Kovaleva, P. Reinke, J. Lieske, J. Fischer, I. Sarrou, D. Komadina, E. Crosas, A. Burkhardt, D. Manstein, A. Meents, H.N. Chapman and D. Oberthuer

223. 3D virtual histology of neuronal tissue by x-ray phase-contrast tomography
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224. Integrated Biology Infrastructure Life-Science Facility at the European XFEL (XBI)
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225. Nuclear inelastic scattering on nitrogenase single crystals and model complexes for NO reaction intermediates in human glutaredoxin
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226. Imaging DNA Compaction During the Cell Cycle by Combined Imaging Techniques
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227. Simulation software for forward projection of peaks in the reciprocal space to the detector of an X-ray diffraction experiment
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228. Mix-and-inject time-resolved serial femtosecond crystallography
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229. Dynamics of complex protein systems studied by X-ray Speckle Visibility Spectroscopy
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230. Enrichment of protein crystal containing insect cells using FACS
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232. Serial crystallography at P11 beamline
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242. Vesicle adhesion and fusion studied by small-angle x-ray scattering
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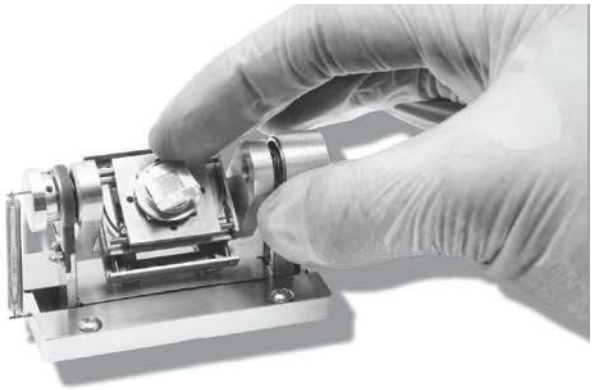

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255. Real-Time Monitoring of π-Stacking of Pentacene on Graphene
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258. An insight into atmospheric degradation processes by mapping local nanoheterogeneities within hybrid polycrystalline perovskite films
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259. Tuning electronic properties of nanogranular silver layers using polymer-template assisted sputter deposition
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260. Piezotronic related strain effects in ZnO microstructures
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262. Grazing incidence X-ray scattering studies of polymer colloidal crystals under dry sintering conditions
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265. Ions at hydrophobic interfaces
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266. Bragg Ptychography Imaging of Phase-Ordering Fe-Al Alloys
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267. Surface-mediated spin-crossover of a low-spin Fe(II) complex probed by NEXAFS
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272. Characterisation of Polymeric Thin Film Systems using GISAXS
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274. Depth profiling of ultrathin ferrite films characterized by angle resolved hard x-ray photoelectron spectroscopy
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276. Magnetic skyrmions in Pt/Co/Ir at zero field
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279. In-situ Meets Operando: Understanding Solar Cell Performance at the Nanoscale through Correlative X-Ray Microscopy
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280. Abnormal Pressure-Induced Photoluminescence Enhancement and Phase Decomposition in Pyrochlore $La_2Sn_2O_7$
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281. Element specific channels in photo excitation of V-doped TiO_2 nanoparticles
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283. Structural change of hafnia (HfO_2) under pressure
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284. Microsecond structural rheology with liquid jets
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285. Electronic Structure of $Fe_{1-x}Ni_x$ Alloys
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286. Composition Dependence of Magnetoresisitance in $Fe_{1-x}Ni_x$ Alloys
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319. X-ray topography is needed! How to identify the growth mechanism of inorganic and protein crystals?
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326. Investigation of organically linked iron oxide nanoparticle supercrystals using SAXS
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329. Study of the luminescence of Eu^{2+} and Eu^{3+} states in $Ca_3Ga_2Ge_3O_{12}$:Eu garnet using synchrotron radiation excitation
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330. Fabrication of toughened superhard polycrystalline materials and elucidation of the toughening mechanism
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331. Time-Dependent Characterization at the Mesoscale: The Matter-Radiation Interactions in Extremes (MaRIE) Project at Los Alamos National Laboratory
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332. Local electronic and crystal structure rearrangement at amorphous - pyrochlore transition in $Ln_2M_2O_7$ (*Ln*=lanthanide, M=Zr, Ti) powders.
A. Menushenkov, V. Popov, B. Gaynanov, F. d'Acapito and A. Puri

333. Phase Transitions and Spall under Shock Compression using X-ray Diffraction and Imaging
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334. Hard X-ray spectroscopy of magnetic thin films for spintronic devices
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335. Pyrolytic graphite electrodes intercalated by $AlCl_4$ anions probed by X-ray tomography and small angle X-ray scattering
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336. Phase contrast tomographic analysis of strain in LCF-loaded Al/Al_2O_3 MMCs
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337. d-d transitions of Ni^{2+} of CPO-27-Ni: a combined UV-Vis, resonant-valence-to-core X-ray emission spectroscopy, and theoretical study
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338. Valence transition in Cu_4InYb captured by DMFT calculations
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339. Structure and dynamics of glass-forming fluids
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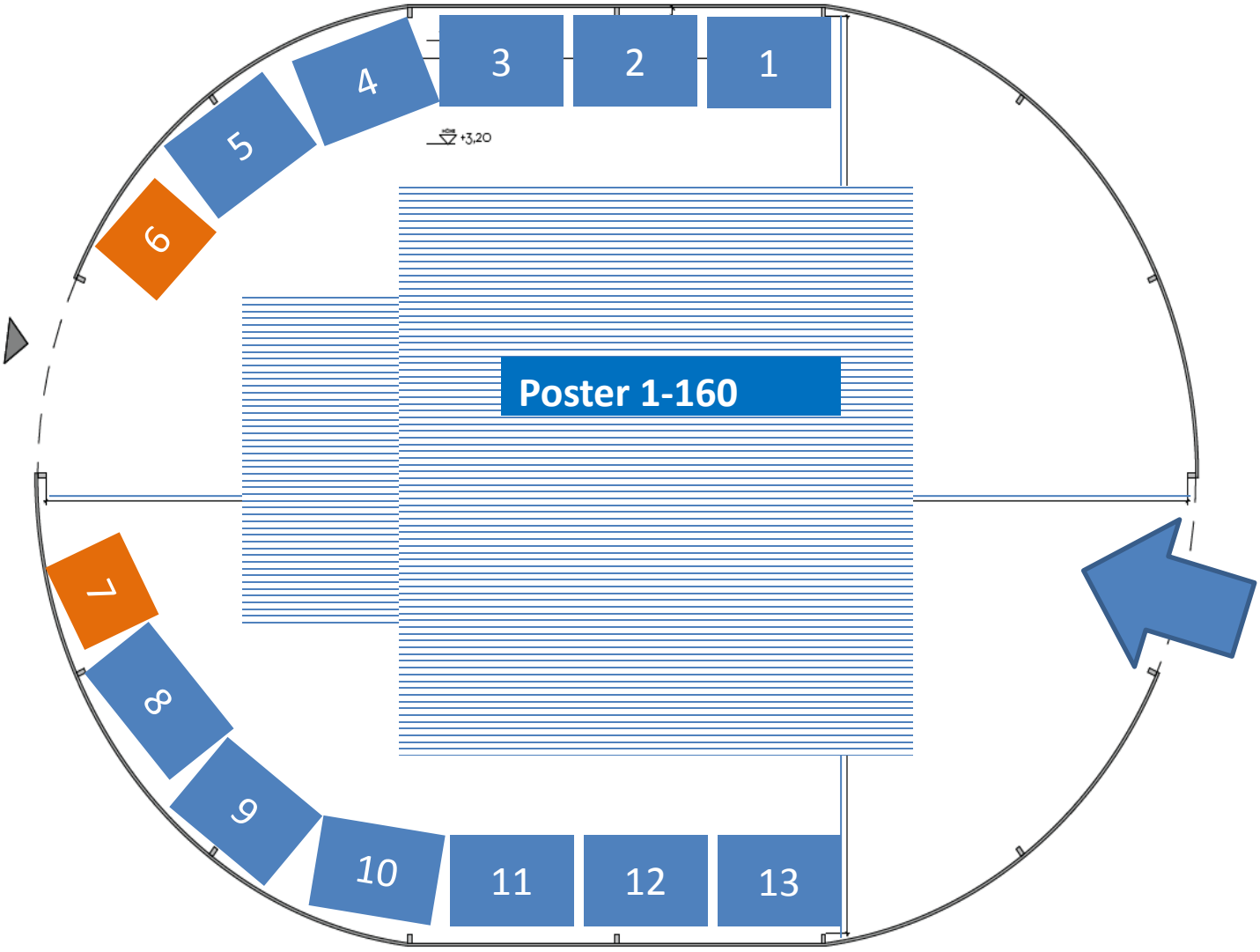
European XFEL Users Meeting 2018
DESY Photon Science Users Meeting 2018

Vendor Exhibition Booths and posters - 26 January 2018

POSTER SESSION (14-17h) and Vendor exhibition (10-18h)
Venue: “Kuppel Hamburg” (dome on the Trabrennbahn Bahrenfeld, opposite to the campus - Luruper Chausse 30)

Entrance tent



European XFEL Users Meeting
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Vendor Exhibition Booths and posters - 26 January 2018

Main tent