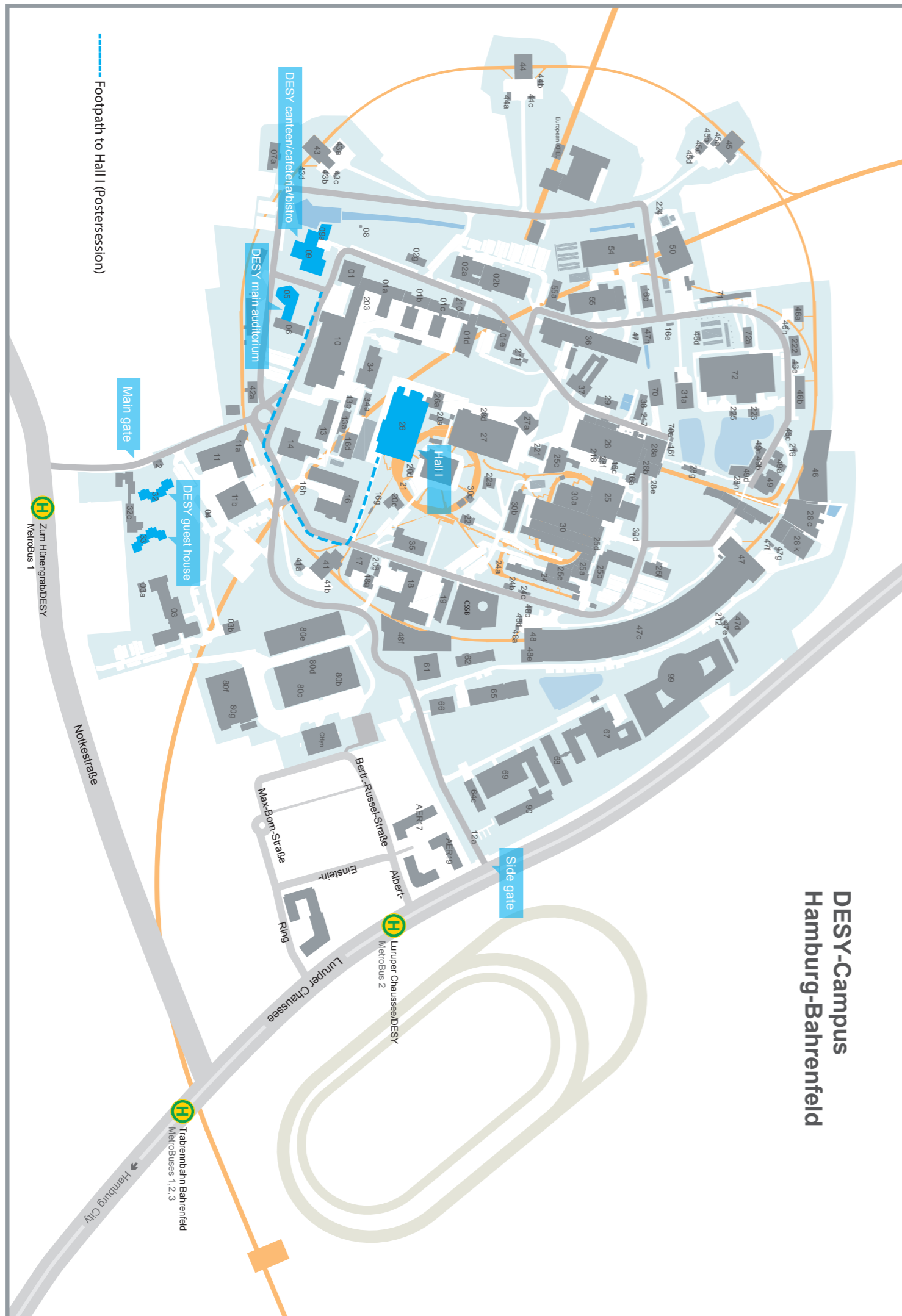


DESY Photon Science Users' Meeting 2017 European XFEL Users' Meeting 2017



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



DESY Photon Science Users' Meeting 2017 European XFEL Users' Meeting 2017

January 25-27, 2017 in Hamburg - DESY Auditorium (Bldg. 5)



Wednesday January 25 **European XFEL Users' Meeting (9:00-14:50 DESY Auditorium)**

08:30–10:00 Registration

10:00–10:20 Opening Session

10:00 Welcome

R. Feidenhans'l *European XFEL*

10:10 Opening Address from the Council Chair

M. M. Nielsen *Techn. Univ. of Denmark*

10:20–12:20 Project update session

Chair: M. M. Nielsen, Techn. Univ. of Denmark

10:20 General Status of the Project

R. Feidenhans'l *European XFEL*

10:50 Electron Accelerator

H. Weise *DESY, Hamburg*

11:20 Detectors at European XFEL

M. Kuster *European XFEL*

11:40 Laser systems for science instruments

M. Lederer *European XFEL*

12:00 FXE instrument

C. Bressler *European XFEL*

12:15 SPB/SFX instrument

A. Mancuso *European XFEL*

12:30–13:50 Lunch break

13:50–14:40 Hard X-ray FELs Science Highlights

Chair: T. Ishikawa, RIKEN SPring-8 Center

13:50 Femtosecond structural dynamics on PYP

M. Schmidt *Univ. of Wisconsin*

14:15 Photoinduced enhancement of the charge density wave amplitude

A. Singer *Univ. of California*

14:40 Coffee break



Bus shuttles to European XFEL site in Schenefeld (every ~20 min. / 14:50-18:00)

15:20 Guided Facility tours (30 min., start every 10 min.) and Project Status Update presented by posters of European XFEL groups

18:30-22:00 European XFEL Dinner Reception for speakers and participants (Schenefeld site, Foyer XHQ)



Bus shuttles to DESY side entrance (every ~20 min. / 19:15-22:30)

Thursday January 26 **FLASH Session | Soft X-ray FEL experiments – jointly organized by DESY and European XFEL (9:00-13:10 DESY Auditorium)**

09:00-09:05 Welcome

Chair: R. Treusch, DESY

E. Weckert *DESY, Hamburg*

09:05-09:35 FLASH – today and tomorrow – status report and future plans

W. Wurth *DESY, Univ. Hamburg*

09:35-09:55 New opportunities at FLASH2

E. Plönjes *DESY, Hamburg*

09:55-10:20 Attosecond interferometry with a SASE FEL

T. Laarmann *DESY, Hamburg*

10:40-11:00 Coffee break

11:00-13:10 Soft X-ray FEL experiments

Chair: R. Feidenhans'l, European XFEL

11:00-11:30 Absorption spectroscopy and control of correlated electron dynamics in small quantum system

C. Ott *MPI Heidelberg*

11:30-12:00 XUV and soft X-ray photoionization studies on gasphase protein and oligonucleotide ions

T. Schlathölder *Univ. of Groningen*

12:00-12:30 X-ray absorption spectroscopy using circular polarization and a self-seeded soft X-ray free-electron laser

D. Higley *SLAC, Stanford*

12:30-13:00 Spatially resolved ultrafast magnetic dynamics initiated at a complex oxide heterointerface

A. Cavalleri *MPI, CFEL*

13:00-13:10 Report of the European Synchrotron User Organism. (ESUO)

J. Pietsch *ESUO Chair, Univ. Siegen*

13:10-14:00 Lunch break

13:00-18:15 Satellite Meetings – Workshops

see next page for details

Thursday January 26 **SATELLITE MEETINGS – WORKSHOPS**

13:00-18:00	X-ray absorption spectroscopy at PETRA III beamlines P64 and P65	<i>CFEL Sem.R. V, Bldg.99</i>
13:00-18:10	SAXS/WAXS/GISAXS-User Workshop @ DESY	<i>DESY FLASH Sem.R., 28c</i>
14:00-18:00	Light-Matter Interaction: Recent Advances in Theory	<i>CFEL Sem.R. II, Bldg. 99</i>
14:00-18:15	7th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III	<i>DESY Sem.R. 4ab, Bldg. 1b</i>
14:00-18:45	Extreme Condition Science at DESY	<i>DESY Sem.R. 109, 25b</i>
13:00-17:30	Tutorial on X-ray Holographic Imaging / Tomography	<i>DESY Sem.R. 2, Bldg. 2</i>
13:00-18:00	New instrument for ultrafast spectroscopy of small quantum objects at FLASH1 and FLASH2	<i>CFEL Sem.R. I, Bldg. 99</i>
14:00-18:00	High energy X-ray diffraction for Physics and Chemistry	<i>DESY Sem.R. BAH1, Bldg. 3</i>
14:00-18:00	High resolution diffraction at solid and liquid interfaces	<i>DESY Sem.R. 456, Bldg.25f</i>
14:00-18:00	Serial Crystallography at FELs and synchrotron sources	<i>DESY Main Auditorium, Bldg. 5</i>
13:00-16:45	Helmholtz-Zentrum Geesthacht GEMS Outstation: Materials Research and High Resolution Imaging	<i>DESY Sem.R. 013, Bldg.66</i>
14:15-18:00	EUCALL Workshop (<i>closed session</i>)	<i>DESY FLASH Sem.R., 28K</i>
19:00	DESY Photon Science Reception for speakers and participants	<i>(DESY canteen, Bldg. 9)</i>

Friday January 27 **DESY Photon Science Users' Meeting (9:00-12:50 DESY Auditorium)**

09:00-09:10	Welcome	Chair: G. Grübel, DESY
09:10-09:50	Photon science at DESY	H. Dosch <i>DESY, Hamburg</i>
09:50-10:20	PETRA III and future outlook	E. Weckert <i>DESY, Hamburg</i>
10:20-10:50	Coffee break	C. Schoer <i>DESY/University of Hamburg</i>
10:50-11:20	DNA origami nanoagents and crystals studied by SAXS	Chair: W. Drube, DESY
11:20-11:50	The inhibition mechanism of human proteasomes	B. Nickel <i>LMU München</i>
11:50-12:20	Correlative X-ray tomography of Aged Fluid-Catalytic-Cracking Catalyst Particles	A. Chari <i>MPI Göttingen</i>
12:20-12:35	Watching aging in organic solar cells - an in-operando study	F. Meirer <i>Utrecht University</i>
12:35-12:50	Report of the DESY Photon Science Users Committee (DPS-UC) Results DPS-UC Election	P. Müller-Buschbaum <i>TU München</i>
12:50-13:00	Report of the ‚Komitee Forschung mit SR‘ (KFS)	P. Müller-Buschbaum <i>DPS-UC Chair, TU München</i>
13:00-14:00	Lunch break	S. Eisebitt <i>KFS Chair, MBI, Berlin</i>
14:00 – 17:00	POSTER SESSION and Vendor exhibition Jointly organized by DESY and European XFEL ("Hall 1", DESY-Bldg. 26)	

Tuesday January 24 **SATELLITE MEETINGS - WORKSHOPS**

09:00-18:00	Status of the HED science instrument & Meeting of the HIBEF user consortium	<i>European XFEL Sem.R. E1.173 (Schenefeld)</i>
10:00-17:30	Soft X-ray Instrumentation SQS and SCS	<i>DESY FLASH Sem.R. , 28c</i>
14:00-18:00	Karabo 2.0: Introduction to the Control and Analysis Framework at the European XFEL	<i>(DESY) Univ.Hamburg, Bldg.90, ZOQ Sem.R.</i>

General Information

Oral and postersession

Oral sessions will be held in the DESY auditorium.

The poster session will be held in the “Halle I” (Bldg. 26)

Sessions Vendor exhibition

The vendor exhibition will take place in the in the “Halle I” (Bldg. 26)

Social events

The European XFEL reception and Site visit will take place on Wednesday, 25 January at the European XFEL Headquarters at Holzkoppel 4, 22869 Schenefeld (see programme).

Bus shuttles DESY -> XFEL are available from 14:50 to 18:00 (every 20 min.) and return from 19:15 to 22:30. Guided facility tours and poster presentations will be provided. Start of reception is at 18:30.

If you plan to go directly, please see http://www.xfel.eu/how_to_reach_us/.



The DESY Photon Science reception will take place on Thursday 26 January at 19:00 in the DESY canteen (Bldg. 9)

DESY WLAN

Name: UserMeeting2017
WPA/WPA2-PSK: wie9ooR3eez9



Organizers

I. Gembalies (European XFEL), M. Kazemi (DESY), M. Kreuzeder (DESY), W. Laasch (DESY), F. Lehmkuhler (DESY), W. Lu (European XFEL), S. Molodtsov (European XFEL), J. Möller (European XFEL), A. Rothkirch (DESY), A. Samanta (DESY), D. Unger (DESY)

Local Information

Cash machine/ATM

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

Meals

Breakfast

If you stay at the DESY guest house you may have breakfast in the DESY cafeteria (opens at 07:00h, Bldg. 9) at your own expenses.

Lunch

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

Supermarkets

LIDL

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

PENNY

From the DESY main gate (Notkestrasse) walk straight down the street “Zum Hünengrab” (700 – 800m).

Opposite to this supermarket you will find a bakery and other shops (drugstore).

DESY Photon Science User Committee Election 2017

Please vote online until
Thursday 26 January, 15:00 h

DOOR.desy.de

I Main sessions
Abstracts of the talks

Femtosecond structural dynamics of photoactive yellow protein

Marius Schmidt

University of Wisconsin-Milwaukee, USA

We established that time-resolved serial femtosecond crystallography (TR-SFX) works at the LCLS [1] and followed the *trans* to *cis* isomerization of the central para-coumaric acid (pCA) chromophore in the photoactive yellow protein in real time [2]. Excited state structural dynamics of the pCA chromophore initiates the *trans* to *cis* isomerization. The transition from the excited state potential energy surface (ES-PES) to the ground state (GS) PES occurs within about 600 fs, after which the configuration of the chromophore is *cis*. By comparing X-ray structures on both the ES-PES and the GS-PES on time scales from 100 fs to 3 ps we structurally characterize the transition through a conical intersection for the first time.

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[1] Tenboer, J., Basu, S., Zatsepin, N., Pande, K., Milathianaki, D., Frank, M., Hunter, M., Boutet, S., Williams, G. J., Koglin, J. E., Oberthuer, D., Heymann, M., Kupitz, C., Conrad, C., Coe, J., Roy-Chowdhury, S., Weierstall, U., James, D., Wang, D., Grant, T., Barty, A., Yefanov, O., Scales, J., Gati, C., Seuring, C., Srajer, V., Henning, R., Schwander, P., Fromme, R., Ourmazd, A., Moffat, K., Van Thor, J. J., Spence, J. C., Fromme, P., Chapman, H. N. & Schmidt, M. (2014). *Science* **346**, 1242-1246.

[2] Pande, K., Hutchison, C. D. M., Groenhof, G., Aquila, A., Robinson, J. S., Tenboer, J., Basu, S., Boutet, S., Deponte, D., Liang, M., White, T., Zatsepin, N., Yefanov, O., Morozov, D., Oberthuer, D., Gati, C., Subramanian, G., James, D., Zhao, Y., Koralek, J., Brayshaw, J., Kupitz, C., Conrad, C., Roy-Chowdhury, S., Coe, J. D., Metz, M., Lourdu Xavier, P., Grant, T. D., Koglin, J., G., K., Fromme, R., Srajer, V., Henning, R., Spence, J. H. C., Ourmazd, A., Schwander, P., Weierstall, U., Frank, M., Fromme, P., Barty, A., Chapman, H. N., Moffat, K., Van Thor, J. J. & Schmidt, M. (2016). *Science* **352**, 725-729.

Photoinduced enhancement of the charge density wave amplitude

Andrej Singer

University of California, San Diego, USA

Symmetry breaking and the emergence of order is one of the most fascinating phenomena in condensed matter physics. It leads to a plethora of intriguing ground states found in antiferromagnets, Mott insulators, superconductors, and density-wave systems. Exploiting states of matter far from equilibrium can provide even more striking routes to symmetry-lowered, ordered states. Here, by utilizing the unique capabilities of the LCLS we demonstrate that moderate photo-excitation in elemental chromium can transiently enhance the charge-density-wave (CDW) order by up to 30% above its equilibrium value, while strong excitation leads to an oscillating, large-amplitude CDW state that persists above the equilibrium transition temperature. By experimentally discerning multiple time scales thus revealing the underlying physics we conclude that both effects result from dynamic electron-phonon interaction. The interaction between these degrees freedom also provides an efficient mechanism to selectively transform a broad excitation of the electronic order into a well-defined, long-lived coherent lattice vibration. This mechanism may be exploited to transiently enhance the order parameter in other systems with coupled degrees of freedom.

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FLASH - today and tomorrow - status report and future plans

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and Center for Free Electron Laser Science, DESY, Notkestr. 85, 22607 Hamburg, Germany

2016 has seen the successful start of user operation of FLASH2 [1]. For the first time we were able to run two user experiments in parallel. In addition to wavelength tuning without changing machine parameters the variable gap undulators installed in FLASH2 allowed a number of experimental tests of new lasing schemes which had been proposed before [2,3]. These tests were extremely successful and schemes like “frequency doubling” and “harmonic lasing self-seeding” should allow to reach shorter wavelength down to the nitrogen K-edge as well as to decrease the spectral bandwidth of the FEL pulses. The overall FLASH performance during user operation was again very good with an uptime exceeding 96%.

In the talk I will review the status of FLASH, present new instrumental developments and some selected recent achievements. Furthermore, I will discuss our plans for the mid- and long-term future of the facility.

[1] B. Faatz, E. Plönjes, et al., S. Schreiber, Simultaneous operation of two soft X-ray free-electron lasers driven by one linear accelerator, *New J. Phys.* 18 (2016) 062002

[2] E.A. Schneidmiller and M.V. Yurkov, Obtaining high degree of circular polarization at x-ray free electron lasers via a reverse undulator taper, *Phys. Rev. ST Accel. Beams* 16 (2013) 110702

[3] E.A. Schneidmiller and M.V. Yurkov, Harmonic lasing in x-ray free electron lasers, *Phys. Rev. ST-AB* 15 (2012) 080702

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New opportunities at FLASH2

Elke Plönjes for the FLASH2 team

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In 2016, first user experiments were conducted at FLASH2 turning FLASH into a multi-user FEL facility. In the experimental hall Kai Siegbahn, which offers space for up to six beamlines, the first two beamlines are now operational:

FL24 features an open port for user provided experimental stations. Presently, this beamline is upgraded with a KB mirror system with bendable mirrors thus enabling variable focal sizes and positions. A grazing-incidence split-and-delay unit designed and constructed by the group of H. Zacharias, Münster University will offer the option of XUV-XUV pump-probe techniques at this beamline. The other beamline FL26 is equipped with a permanent endstation – the reaction microscope REMI provided by the group of R. Moshhammer, MPIK Heidelberg. It will also be upgraded with a grazing-incidence split-and-delay unit in summer 2017. The optical pump-probe laser will be installed by the end of 2017, while a THz undulator for XUV-THz pump-probe experiments is under development for installation in 2018.

In the past year, significant achievements have been made in the exploration of the FLASH2 parameter range spanning the wavelength region of 4-90 nm and reaching peak pulse intensities of up to 1 mJ. New schemes to reach fundamental wavelengths below the nitrogen K-edge and higher harmonics in the water window were demonstrated. Online diagnostics - which are mostly pulse resolved - for beam intensity, position, wavelength, wave front, and pulse length, which have been to a large extent developed at FLASH1 over the past decade, have been optimized for FLASH2.

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Attosecond interferometry with a SASE FEL

Sergey Usenko^{1,2}, Andreas Przystawik¹, Markus Jakob^{2,3}, Leslie Lamberto Lazzarino³,
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Light-phase-sensitive techniques such as coherent multidimensional spectroscopy are well-established in a broad spectral range, already spanning from radio-frequencies in nuclear magnetic resonance spectroscopy to nonlinear optics with table-top lasers in the visible to ultraviolet spectral range. Here, the ability to tailor the phases of electromagnetic waves with high precision is essential. In the present contribution light-phase control on the attosecond timescale ($1 \text{ as} = 10^{-18} \text{ s}$) is achieved in a Michelson-type all-reflective interferometric autocorrelator generating coherent pulse replicas in the limit of short wavelength. The resulting fringe contrast monitors the field interference when varying the relative phase within the optical cycle, i.e. the free-electron laser (FEL) light wave oscillation with a period of $129 \pm 4 \text{ as}$ at a wavelength of 38 nm. The successful transfer of a powerful table-top method towards FEL science and technology paves the way towards utilization of advanced nonlinear methodologies even at partially coherent soft X-ray FEL sources making use of self-amplified spontaneous emission.

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Absorption spectroscopy and control of correlated electron dynamics in small quantum systems

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Absorption spectroscopy is a technique to directly measure the intrinsic optical response of a system, providing a characteristic “fingerprint” of the target under investigation. Especially in the extreme ultraviolet (XUV) and x-ray spectral domain, with access to core transitions, a distinct element specificity and a high sensitivity to the chemical environment can be listed as key advantages. Furthermore, even the intrinsic femtosecond and attosecond timescale of the (multi-)electron dynamics that are associated to such transitions are within reach, by using either table-top high-harmonic generation sources or light generated at XUV/x-ray free-electron lasers. While high-precision line profiles can be routinely accessed at synchrotron facilities, with lifetime information already obtained from the observed line width, the use of previously listed new light sources for absorption spectroscopy opens up a completely new access to directly measure and control the underlying light-matter interaction in weak and strong fields. With a precise understanding of the line profiles and most importantly their asymmetry, correlated multi-electron dynamics are directly accessible, encoding multi-channel interactions of different electron configurations [1], commonly known as Fano absorption line shapes. Hereby, using strong and short flashes of light to induce couplings between multi-channel transitions, a deeper understanding and control of such multi-electron dynamics can be gained. This talk surveys recent own progress in this direction, providing an intuitive time-domain approach to put both symmetric Lorentzian and asymmetric Fano absorption profiles on common grounds [2], with a control knob to finely tune two-electron dynamics in helium in ultrashort optical fields [3]. Furthermore, the time-resolved measurement of the buildup of an asymmetric Fano resonance allows one to gain new insight into the nature of these resonances [4]. As an outlook, strongly driving such autoionizing states with free-electron lasers directly in the XUV and x-ray domain may open up a new level of understanding of the underlying transition dynamics, which also can be regarded as a fundamental example of a chemically important transition state during the process of an ionizing reaction pathway, adding a novel time-domain perspective to the diverse toolbox of core hole spectroscopies.

[1] U. Fano, Phys. Rev. 124, 1866 (1961).

[2] C. Ott, A. Kaldun, P. Raith, K. Meyer, M. Laux, J. Evers, C. H. Keitel, C. H. Greene, T. Pfeifer, Science 340, 716 (2013).

[3] C. Ott, A. Kaldun, L. Argenti, P. Raith, K. Meyer, M. Laux, Y. Zhang, A. Blättermann, S. Hagstotz, T. Ding, R. Heck, J. Madronero, F. Martín, T. Pfeifer, Nature 516, 374 (2014).

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XUV and soft X-ray photoionization studies on gas-phase protein and oligonucleotide ions

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The investigation of complex biological molecules by means of scattering or absorption of energetic photons from high brilliance light sources is a very powerful approach to address the molecules' chemical and electronic structure and dynamics. Established techniques such as X-ray photoelectron spectroscopy (XPS) or near edge X-ray absorption fine structure (NEXAFS) spectroscopy involve small absorption cross sections which usually dictate the use of dense condensed-phase targets. To investigate biomolecular photoionization in the gas-phase, we employ a combination of electrospray ionization (ESI) and radiofrequency (RF) ion guiding and trapping. K-edge soft X-ray photoionization of the protonated peptide leucine enkephalin (555 Da, 5 amino acid residues) leads almost exclusively to extensive fragmentation dominated by loss of small amino acid sidechains [1]. This is understood in a framework of ionization induced fast dissociation through repulsive states before internal vibrational redistribution (IVR) of the excitation energy [2]. For large proteins such as multiply protonated cytochrome c (~12 kDa, 104 residues), in contrast mainly non-dissociative single and double ionization is observed [3]. As the heat capacity is much larger for cytochrome c than for leucine enkephalin, the internal temperature after photoabsorption is much lower. However, fast dissociation leading to sidechain loss is not fully suppressed, even in the largest proteins under study. The transition between both size and temperature regimes is gradual, with a co-existence of backbone scission, sidechain loss and non-dissociative ionization for intermediate size systems with a few kDa mass [4].

Rather than varying protein size, the internal temperature of a protein upon soft X-ray photoabsorption can be varied by the number of absorbed photons. To this end, we have used FLASH to investigate photofragmentation of ubiquitin ions in intense 90 eV / 70 fs pulses as a function of intensity [5]. With increasing intensity, sidechain fragment yields increase linearly while backbone scission remains negligible. Ionization clearly triggers a localized molecular response that occurs before the excitation energy equilibrates. Consistent with this interpretation, the effect is barely affected by the initial charge state of the ubiquitin. The fragmentation patterns of sixfold deprotonated and tenfold protonated ubiquitin turn out to be very similar. Ubiquitin thus responds to EUV multiphoton ionization as an ensemble of small peptides.

Our most recent ongoing experiments address the excitation and structural dynamics in DNA oligonucleotides as a function of DNA sequence.

[1] O. Gonzalez-Magaña, G. Reitsma, M. Tiemens, L. Boschman, R. Hoekstra, T. Schlathölter, *J. Phys. Chem. A* 2012, 116, 10745

[2] S. Bari, O. Gonzalez-Magaña, G. Reitsma, R. Hoekstra, J. Werner, S. Schippers, T. Schlathölter, *J. Chem. Phys.* 2011, 134, 024314

[3] A. R. Milosavljević, F. Canon, C. Nicolas, C. M. L. Nahon, a. A. Giuliani, *J. Phys. Chem. Lett.* 2012, 3, 1191

[4] D. Egorov, L. Schwob, M. Lalonde, R. Hoekstra and T. Schlathölter, *Phys. Chem. Chem. Phys.* 2016, 18, 26213

[5] T. Schlathölter, G. Reitsma, D. Egorov, O. Gonzalez-Magaña, S. Bari, L. Boschman, E. Bodewits, K. Schnorr, G. Schmid, C. D. Schröter, R. Moshhammer, R. Hoekstra, *Angew. Chem. Int. Ed.* 2016, 55, 10741

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Soft X-ray Absorption Spectroscopy using Circular Polarization at LCLS

Daniel Higley¹, Alex Reid¹, Loïc Le Guyader¹, Georgi Dakovski¹, Joe Chen¹, Konstantin Hirsch¹, Emmanuelle Jal¹, Edwin Yuan¹, Tianmin Liu¹, Tyler Chase¹, Patrick Granitzka¹, Alberto Lutman¹, James MacArthur¹, Giacomo Coslovich¹, Olav Hellwig², Pádraic Shafer³, Matteo Pancaldi⁴, Stefano Bonetti⁴, Hermann Dürr¹, Joachim Stöhr¹ and William F. Schlotter¹

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Circular polarization is required for certain X-ray techniques. One such technique is X-ray magnetic circular dichroism spectroscopy (XMCD), which is frequently used at storage ring light sources to probe magnetic properties of matter with elemental specificity, as well as resolve magnetic properties into their separate spin and orbital moment components. XMCD's requirement of circular polarization is now fulfilled at the Linac Coherent Light Source (LCLS) X-ray free electron laser thanks to a recently installed variable polarization "delta" undulator. Using this and other advances, we can now perform XMCD with the femtosecond and 100s of uJ pulses of LCLS. Doing so opens up new kinds of XMCD studies, which we show some examples of. (1) We measured the ultrafast all-optical switching of a GdFeCo alloy with unprecedented sensitivity. This confirmed the existence of a transient ferromagnetic state mediating the switching, as well as revealed previously unseen aspects of the fluence dependence of magnetization dynamics near the switching fluence. (2) We simultaneously followed the ultrafast magnetic and electronic dynamics initiated by an optical pump pulse in a Co/Pd multilayer. This was accomplished through XMCD over the Co L₃ edge and revealed ultrafast changes in the occupations of states near the Fermi level and demagnetization. (3) We discovered large nonlinearities in the XMCD and x-ray absorption near the Co L₃ edge of a Co/Pd multilayer. These nonlinearities qualitatively follow the spectral changes induced by an optical pump pulse in Co/Pd. We compare these changes to those expected from the X-ray-induced secondary electron cascade and subsequent demagnetization. The success of these early results is particularly exciting given the imminent improvements for XMCD at XFELs. Through more efficient use of the abundant photons provided in each XFEL pulse and use of upcoming high repetition rate XFELs, more than an order of magnitude improvement in sensitivity is possible. These developments will extend the studies of fine details of the magnetic properties of materials, which are commonplace at storage ring light sources, to the ultrafast domain.

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Spatially resolved ultrafast magnetic dynamics initiated at a complex oxide heterointerface

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²*Centre for Free Electron Laser Science, University of Hamburg*

³*Department of Physics, University of Oxford*

In this talk, I will discuss recent work in which the lattice of complex oxide heterostructures is controlled coherently with THz frequency pulses. The interface couples the optically driven substrate with a material across it, in which some of the properties are dynamically changed. I will report experiments that combine measurements of the ultrafast optical conductivity with femtosecond soft and hard x-ray probing with Free Electron Laser pulses. The dynamical structure, the changes in charge and magnetic order are measured as they propagate into the material.

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DNA origami nanoagents and crystals studied by SAXS

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DNA origami nanostructures enable the self-assembly of arbitrarily shaped objects with unprecedented accuracy. We present high precision measurements of shape and internal structure of three prototypic DNA origami structures using synchrotron small angle X-ray scattering. Sheet-, brick- and cylinder-shaped DNA constructs were assembled and the shape factors determined with Ångström resolution. Electrostatic swelling of shape cross section and inter-helical DNA spacing of the DNA origami structures was observed with decreasing MgCl_2 concentration. The structures tolerate up to 10% inter-helical expansion before they disintegrate. In contrast, the cylinder-shaped structures show no thermal expansion with increasing temperature in a wide temperature window before they abruptly melt above 50°C . Our present activities focus on building up 3D-crystals from DNA origami building blocks. By DNA addressing, we envision precise decoration of such crystals with biomolecules and quantum dots.

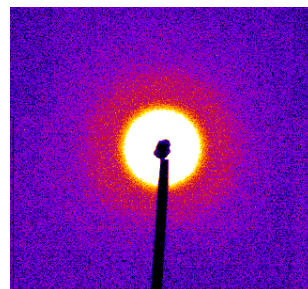


Figure 1. Schematic of a DNA origami 24 helix bundle and the 2D SAXS signal.

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The inhibition mechanism of human proteasomes

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The proteasome is a validated target for anti-cancer therapy and proteasome inhibition is employed in the clinic for the treatment of tumors and hematological malignancies. Here, we describe crystal structures of the native human 20S proteasome and its complexes with inhibitors, which are either drugs approved for cancer treatment or are in clinical trials. The structures were determined at unprecedented resolutions of below 2 Å resolution as a consequence of a variety of technical innovations in proteasome purification, crystallization and X-ray data collection. The 20S proteasome structures allow direct observation of inhibition mechanisms that differ from earlier models determined at lower resolution. Collectively, the high-resolution structures provide new insights into the catalytic mechanisms of inhibition and necessitate a revised description of the proteasome active site. Knowledge about inhibition mechanisms provides insights into peptide hydrolysis and can guide strategies for the development of next-generation proteasome-based cancer therapeutics.

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Correlative X-ray tomography of aged fluid-catalytic-cracking catalyst particles

Florian Meirer

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Modern X-ray imaging techniques allow for the combination of high spatial resolution, a large field of view, short dwell times, and the capability to obtain spectroscopic information. This has opened the door to high-resolution studies correlating chemistry and morphology of, for example, whole catalyst particles used in fluid catalytic cracking (FCC).

FCC is an important process in the petrochemical industry, accounting for 40-45% of worldwide gasoline production. In FCC, catalyst particles are used to crack large hydrocarbon fractions into more valuable materials, such as gasoline and propylene [1]. During operation FCC catalyst particles accumulate metals (e.g. Fe, Ni, V, Ca, Na) that have been related to catalyst deactivation. However, detailed knowledge about metal deposition mechanisms and their effects on particle morphology and chemistry is limited.

In this presentation I will first very briefly summarize the main results obtained during our recent studies of individual FCC catalyst particles using synchrotron based hard X-ray full field transmission X-ray microscopy (TXM) [2-4,6], hard X-ray fluorescence (XRF) tomography [5,6], soft X-ray ptychographic imaging [7], and soft X-ray scanning transmission X-ray microscopy [8]. I will then discuss in more detail the latest results obtained by correlative X-ray microscopy, i.e. combining XRF tomography with (1) TXM tomography [6] and (2) with hard X-ray ptychography tomography.

References

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- [2] F. Meirer, D.T. Morris, S. Kalirai, Y. Liu, J.C. Andrews, B.M. Weckhuysen, *J. Am. Chem. Soc.* **137**, 102–105 (2015).
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Watching aging in organic solar cells - an in-operando study

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In terms of large scale usability, one of the major challenges for organic photovoltaic cells is to overcome their relatively short lifetime, as compared to inorganic counterparts. To gain a deeper understanding of organic solar cell degradation with respect to changes in the active layer nano-morphology, we present an in-situ study on model polymer-fullerene solar cells during the first hours of operation. It reveals information on both, its evolving current-voltage characteristics and active layer nano-morphology. For that purpose, grazing incidence small angle X-ray scattering (GISAXS) measurements and current-voltage (IV) tracking of an operating solar cell are performed simultaneously [1-3].

In the in-operando studies we investigate different types of polymer solar cells. In case of P3HT:PCBM solar cells in standard device geometry domains on the nanometer scale within the device's active layer are found to grow and drift apart during operation while the short circuit-current decreases. Based on Monte-Carlo simulation, these nano-morphological changes in the active layer are found to fully explain the decrease of the short-circuit current with time [1]. In contrast, in an inverted device geometry a high stability of the solar cells is caused by absence of such morphological changes [2]. In case of low-band gap polymers such as PCPDTBT the used solvent additive gives rise to a different degradation mechanism. The active layer morphology undergoes domain shrinkage. The smaller domains lose their connection and the initially well interpenetrating network gets deteriorated. As a consequence, charge carriers are more likely trapped in isolated domains, which amplifies recombination and lowers the fill factor of the devices [3].

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II Programmes Satellite Meetings



X-ray absorption spectroscopy at PETRA III Beamlines P64 and 65

Thursday, 26 January 2017

CFEL Bldg. 99, Seminar Room V

Beamline P65 went into full user operation in June 2016, and P64 got first beam in May 2016. The satellite workshop shall give an overview about the current status of both beamlines P64 and P65, and the associated projects. 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

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wolfgang.caliebe@desy.de

PROGRAMME

Session 1: Instrumentation

Chair: Wolfgang Caliebe

13:00	Welcome	Wolfgang Caliebe	DESY
13:05	Status of P64	Vadim Murzin	DESY
13:25	Status and preliminary results of the high-resolution XES Spectrometer at P64	Aleksandr Kalinko	Univ. Paderborn
13:45	P65, the first year with user operation	Edmund Welter	DESY
14:10	Taurus, Spock, Tango, Sardana – Software at the EXAFS-Beamlines	Roman Chernikov	DESY
14:30	Discussion: What is required for future experiments? Optics, detectors and software		

15:00 Coffee break

Session 2: Experimental Results

Chair: Edmund Welter

15:30	Oxygen 2s-spectroscopy at P01	Georg Spiekermann	Univ. Potsdam
15:50	First in operando studies at beamline P65	Matthias Steib	TU München
16:10	First in situ and operando X-ray absorption spectroscopic catalyst characterization at P64	Andreas Gänzler	KIT
16:30	UiO-66 to MIL-140A - a combined XRD and XAFS analysis	Niclas Heidenreich	CAU Kiel
16:50	EXAFS of Silver Clusters in Ionic Liquids	Stefanie Röse	TU Dortmund
17:10	In Situ X-ray Absorption Studies on Electrode Materials for Rechargeable Lithium and Sodium Ion Batteries: An Overview of Measurement Time at P65 Beamline	Geethu Balachandran	KIT
17:30	Surface Spectroscopy in the DESY NanoLab	Heshmat Noei	DESY
	Discussion: Sample environments and preparation lab		
18:00	End of meeting		



Tutorial on X-ray Holographic Imaging / Tomography

Thursday, 26 January 2017

Bldg. 2, Seminar Room 2

New (coherent) X-ray imaging capabilities have been developed, implemented and exploited at several instruments of PETRA III, e.g. at the beamline P05 (HZG) and the P10-GINIX setup (built by the University of Göttingen). Some of the interesting options include high resolution near-field imaging in the holographic regime and tomography. These developments led to the highest resolution images recorded in full-field in-line holography (Bartels et al., PRL 114, 048103, 2015) as well as to novel opportunities for tomographic imaging of biological cells and tissues (Krenkel et al., Scientific Reports 5, 9973, 2015). The full field micro tomography setup offers high-throughput user experiments in absorption mode and opens up unique possibilities in phase contrast mode (Stebner et al., Scientific Reports 6, 34352, 2016). In addition the nanotomography experiment is now in user operation offering full field x-ray microscopy at high spatial resolution (Ogurreck et al., JSR 23, 2016).

The first part of this tutorial workshop will give an introduction to both techniques and present the current instrumentation available at P05 and P10. Afterwards presentations will demonstrate the current capabilities and limitations of both instruments.

Organisers: M. Sprung, I. Greving

Contact: michael.sprung@desy.de

PROGRAMME

Session 1: Tomography				<i>Chair: M. Sprung</i>
13:00	Welcome			DESY/HZG
13:10	Basics of imaging and tomography (40 + 5)	I. Greving		HZG
13:55	Imaging at the Beamline P05 (25 + 5)	F. Wilde		HZG
14:25	Examples and Applications (15 + 5)	F. Wilde		HZG
14:45	Coffee break			
Session 2: Holographic Imaging				<i>Chair: M. Sprung</i>
15:15	Tutorial on Holographic Imaging (40+5)	T. Salditt		Univ. Göttingen
16:00	Imaging at P10-GINIX (25+5)	M. Osterhoff		Univ. Göttingen
16:30	Tomography of neural tissues (15+5)	M. Töpperwien		Univ. Göttingen
16:50	to be announced	M. Vassholz or K. Giewekemeyer		Univ. Göttingen European XFEL

SATELLITE WORKSHOP - Photon Science



High energy X-ray diffraction for Physics and Chemistry

Thursday, 26 January 2017

Bldg. 3, Seminar Room BAH1

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. We invite workshop participants to give a talk on their work in the topics of

- powder or single crystal diffraction
- surface and interface diffraction
- amorphous and nanostructured materials

Organiser: Uta Rütt

Contact: uta.ruett@desy.de

PROGRAMME

14:00	Status Powder Diffraction Beamline P02.1,	Martin Etter	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	Uta Ruett	DESY
15:30	<i>Coffee break</i>		
16:00	Atomic short range order of functional thin film	Ann-Christin Dippel	DESY
16:30	Melting and solidification of bulk metallic glasses	Olga Shuleshova	IFW Dresden
17:00	In situ oxide film growth by MBE	Joachim Wollschläger	Univ. Osnabrück
17:30	In Situ Studies on Phase Transitions of $\text{Al}(\text{acac})_3$	Huayna Terraschke	Univ. Kiel
18:00	<i>End of meeting</i>		



Serial Crystallography at FELs and synchrotron sources

Thursday, 26 January 2017

DESY Auditorium, Bldg. 5

Serial Femtosecond X-ray crystallography (SFX) at X-ray Free Electron Lasers (XFELs) has changed the way crystallographic data can be collected. Instead of investigating one or a few large crystals, still images from hundreds to hundred of thousands of crystals are collected in series. Recently, the technique of serial crystallography has also been very successfully applied at synchrotron sources. In addition to determinations of ground state structures from micro- and nano-crystals, an important potential of serial crystallography is studying kinetics of irreversible enzyme reactions. Dynamic events can be induced in different ways; such as laser excitation, microfluidic mixing, temperature jumps, cleavage of caged compounds, and others.

With the European XFEL and the PETRA III storage ring the Hamburg metropolitan area offers excellent opportunities for serial crystallography experiments. During this workshop, application experts will present their latest results along with facility experts showcasing the experimental opportunities at the SPB/SFX instrument of the European XFEL and the PETRA III biology beamlines.

Organisers: A. Mancuso, A. Meents, J. Schulz, H. Chapman

Contact: alke.meents@desy.de

PROGRAMME

14:00	Welcome	Alke Meents	DESY / CFEL
14:10	Capturing the structure of a biochemical interaction intermediate state of a riboswitch in real time using an XFEL	Yun-Xing Wang	NIH / National Cancer Institute
14:40	Serial femtosecond crystallography pump probe experiments	Ilme Schlichting	Max Planck Society
15:10	A molecular movie of the bacteriorhodopsin photocycle on the nanosecond to millisecond time scale	Antoine Royant	ESRF / Institut de Biologie Structurale
15:40	Beyond the Braggs - Getting more from protein crystallography	Oleksandr Yefanov	DESY / CFEL
16:10	<i>Coffee break</i>		
16:40	Opportunities for serial crystallography using the SPB/SFX instrument at the European XFEL	Adrian Mancuso	European XFEL
17:10	Opportunities for Serial Crystallography at beamline P11 at PETRA III	Anja Burkhardt	DESY
17:30	Workflows for serial crystallography on beamline P14	Johanna Kallio	EMBL Hamburg

SATELLITE WORKSHOP - Photon Science



Light-Matter Interaction: Recent Advances in Theory

Thursday, 26 January 2017

CFEL Bldg. 99, Seminar Room 2

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.

Organisers: Beata Ziaja-Motyka (Executive) ,
Sang-Kil Son, Robin Santra

Contact: beata.ziaja-motyka@cfel.de

PROGRAMME

	Session 1		<i>Chair: Sang-Kil Son</i>
14:00	Welcome adress	Robin Santra	(CFEL, DESY)
14:15	Theoretical treatment of molecules in ultrashort intense laser pulses: from molecular hydrogen to ammonia.	Alejandro Saenz	(Humboldt Univ., Germany)
14:45	High-intensity x-ray induced radiation damage in proteins.	Stefan Hau-Riege	(LLNL, USA)
15:15	Modeling of X-ray induced non-equilibrium dynamics of matter.	Zoltan Jurek	(CFEL, DESY)
15:45	Coffee break		
	Session 2		<i>Chair: Beata Ziaja-Motyka</i>
16:15	Simulating Thomson scattering from non-equilibrium plasmas.	Thomas Bornath	(Rostock Univ., Germany)
16:45	Recent developments in Time-Dependent Density Functional Theory of warm dense matter.	Andrew D. Baczewski	(Sandia Nat. Lab., USA)
17:15	Structural analysis by X-ray intensity angular cross correlations.	Ruslan Kurta	(European XFEL)
17:45	Closing remarks	Beata Ziaja	(CFEL, DESY)
17:55	End of meeting		

SATELLITE WORKSHOP - Photon Science



High resolution diffraction at solid and liquid interfaces

Thursday, 26 January 2017

Bldg. 25f, Seminar Room 456

This workshop will address current and potential users working in the field of diffraction and scattering on surface, interface, and thin film structures.

The high resolution diffraction at solid and liquid interfaces workshop will focus on recent and future activities at the P08 High Resolution Diffraction Beamline using the high resolution Kohzu diffractometer and the Liquid Scattering Apparatus (LISA). In the workshop we would like to bring the user communities of both instruments together to discuss current and future possibilities at P08 and to enhance communication within the user community.

Organisers: Florian Bertram, Bridget Murphy

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murphy@physik.uni-kiel.de

PROGRAMME

	Session 1		<i>Chair: Florian Bertram</i>
14:00	Welcome		
14:10	P08 News and Highlights	Florian Bertram	DESY
14:35	LISA News and Highlights	Bridget Murphy	CAU Kiel
15:00	X-Ray Reflectivity Studies of Ionic Liquid Interfaces	Markus Mezger	MPI for Polymer Research Mainz
15:35	Structure and strain of epitaxial ultrathin nickel ferrite films on MgO(001) and SrTiO ₃ (001)	Joachim Wollschläger	Universität Osnabrück
16:00	<i>Coffee break</i>		
	Session 2		<i>Chair: Bridget Murphy</i>
16:20	Confined Liquids at P08	Milena Lippmann	DESY
16:45	Interaction Between Host Defence Peptides and Mycobacteria	Thomas Gutschmann	FZ Borstel
17:10	Potential induced nucleation of PbFBr crystals at the mercury-electrolyte interface	Sven Festersen	CAU Kiel
17:35	Poster Clip Session		
18:00	Conclusions		

SATELLITE WORKSHOP - Photon Science



SAXS/WAXS/GISAXS user workshop@ DESY

Thursday, 26 January 2017

FLASH Seminar Room, Bldg. 28c

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: Rainer Gehrke, Stephan Roth

Contact: rainer.gehrke@desy.de

PROGRAMME

	Session 1: Welcome & Status of SAXS/WAXS/GISAXS at DESY		<i>Chair: Matthias Schwartzkopf</i>
13:00	Welcome	Stephan Roth	DESY/KTH
13:10	Progress at P03/MiNaXS	Stephan Roth	DESY/KTH
	Session 2: In-situ investigation of fabrication processes: Vacuum deposition		<i>Chair: Stephan V. Roth</i>
13:30	Flexible titania electrodes for lithium-ion batteries	Ezzeldin Metwalli	TUM
13:50	Real time investigation of optical properties and morphology during the co-sputter deposition of Au/Ag nanoparticles	Deniza Chekrygina	UHH
	Session 3: Energy conversion and storage		<i>Chair: Stephan V. Roth</i>
14:10	Water-processable hybrid solar cells - in situ studies of particular fabrication steps	Volker Körstgens	TUM
14:30	Synchrotron WAXS measurements on lithium intercalated carbon fibres for structural battery applications	Johan Hagberg	KTH
14:50	Morphological degradation in low bandgap polymer solar cells – an in operando study	Peter Müller-Buschbaum	TUM
15:10	Coffee break		
	Session 4: μfluidics		<i>Chair: Matthias Schwartzkopf</i>
15:50	μ fluidics and cellulose	Daniel Söderberg	KTH
16:10	Structured particles by means of fluidized bed technology	Stephan Heinrich	TUHH
16:30	Flow-assisted assembly of nanostructured protein microfibers	Christofer Lendel	KTH
16:50	Microfluidics at High Intensity X-Ray Sources - Latest Results	Martin Trebbin	UHH
	Session 5: Soft matter - structure formation and deformation		<i>Chair: Matthias Schwartzkopf</i>
17:10	Soft matter in Hard Confinement: Liquid condensation and liquid crystalline order in nanopores as explored by SAXS	Patrick Huber	TUHH
17:30	Melting and solidification of polyurethane. The influence of nucleating agents on morphology evolution.	Almut Stribeck	UHH
17:50	WAXS- and SAXS-measurements with high time resolution during quick deformation combined with thermography	Konrad Schneider	IPF
18:10	End of Satellite Meeting		

SATELLITE WORKSHOP - Photon Science



Extreme Conditions Research at DESY

Thursday, 26 January 2017

Bldg. 25b, Seminar Room 109

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 temperatures can be performed at the Extreme Conditions Beamline (P02.2) at PETRA III and in future at the Large Volume Press beamline (P61.1) while research in the WDM regime can be performed at FLASH. However, Extreme Conditions Research is also performed more frequently at other beamline 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. Furthermore, we are starting to think about the possibilities that a diffraction limited storage ring such as proposed for PETRA IV might offer in the not so far future. Within this satellite meeting we will present ongoing research from different user groups at the different beamline of PETRA III and FLASH, give a status report on the DAC platform at the European XFEL and give an outlook on first scientific ideas that make PETRA IV unique among other small emittance 3rd generation light sources.

Organisers: Hanns-Peter Liermann & Sven Toleikis

Contact: hanns-peter.liermann@desy.de

PROGRAMME

14:00	Welcome	S.Toleikis, H.P. Liermann	DESY
	Session 1: Extreme Conditions Research at PETRA III		<i>Chair: Hanns-Peter Liermann</i>
14:10	Overview of the current capabilities of the ECB and ECSI	K. Glazyrin	DESY
14:25	Single Crystal Diffraction at High-Pressure and - Temperatures in the Laser Heated DAC	L. Dubrovinsky	BGI
14:40	Conducting Experiments Beyond 4 Mbar with the dsDAC at P02.2 and P06	L. Dubrovinsky	BGI
14:55	Coffee break		
15:20	High-Pressure, Low-Temperature work at P09	L. Veiga	DESY
15:35	High-Pressure, Low-Temperature work at P02.2	K. Glazyrin	DESY
15:50	Work in the Paris Edinburg Press at P02.1	M. Wilke	Uni. Potsdam
16:05	Radial Diffraction Experiments at the ECB	J. Immoor H. Marquardt	BGI
16:20	Phase Transition Kinetic Studies on PPv	Ch. Langrand S. Merkel	Univ. Lille
16:35	Offline synthesis with the 6 piston LVP	T. Katsura	BGI
17:00	Coffee break		
	Session 2: Extreme Conditions Research at FLASH		<i>Chair: S. Toleikis</i>
17:20	AC conductivity in WDM gold	S. Glenzer	SLAC
17:35	Electrical and thermal properties of isochorically heated water	S. Sperling	European XFEL
17:50	Ultra-fast solid to solid phase transition in diamond	M. Prandolini	HI Jena
	Session 3: Future Development for Extreme Conditions Research at DESY		<i>Chair: K. Glazyrin</i>
18:05	Status of the TDR for DAC experiments at the HED instrument of the European XFEL	H.P. Liermann	DESY
18:20	Future Prospects for Extreme Conditions Research at PETRA IV	H.P. Liermann	DESY
18:35	Close-out	S. Toleikis H. P. Liermann	DESY
18:45	End of Satellite Meeting		

SATELLITE WORKSHOP - Photon Science



7th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III

Thursday, 26 January 2017

Bldg. 1, Seminar Room 4b

The workshop covers X-ray microscopy at PETRA III with special emphasis on applications in biology and chemistry. It is held for the 7th time and brings together scientists from biology, chemistry, and X-ray microscopy. This satellite workshop covers some recent methodological and instrumental developments at PETRA III and the DESY NanoLab as well as some scientific applications. 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, Ch. Schroer

Contact: gerald.falkenberg@desy.de

PROGRAMME

			<i>Chair: G. Falkenberg</i>
14:00	Welcome & X-ray Microscopy Today and at PETRA IV	Christian Schroer	DESY/UHH
14:30	Continuous Scanning & Fast Data Acquisition at P06	Jan Garrevoet	DESY
14:50	Upgrade of the Hard X-Ray Nanoprobe (PtyNAMi)	Andreas Schropp	DESY
15:10	Complementary Nano- and Micro-Imaging at DESY NanoLab	Thomas Keller	DESY
15:30	Operando Investigation of Single Pt Catalyst Nanoparticles	Marie Ingrid Richard	ESRF
16:00	<i>Coffee break</i>		
			<i>Chair: Ch. Schroer</i>
16:30	Correlative Biological Imaging using Simultaneous Ptychography and X-ray Fluorescence	Karolina Stachnik	DESY
17:00	The Determination of Element Distribution in Plants by Transport Proteins	Stefanie Höller	Univ. Halle-Wittenberg
17:30	Nano-Diffraction from Coupled Organic-Inorganic Nanostructures (COINs)	Frank Schreiber	Univ. Tübingen
18:00	Closing Remarks & End of Meeting		



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

Thursday, 26 January 2017

Bldg. 66, Seminar Room 013

The 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 2017 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

Session 1: Diffraction			
13:00	Welcome	Martin Müller	<i>Chair: P. Staron</i> HZG, Inst. of Materials Research
13:10	Status of HEMS and the new white-beam beamline	Peter Staron	HZG, Inst. of Materials Research
13:25	High-energy X-ray diffraction as a probe of current distribution in Li-ion batteries	Anatoliy Senyshyn	TU Munich/MLZ
13:45	In situ diffraction experiments during high-pressure torsion deformation	Erhard Schafler	Univ. Vienna, Faculty of Physics
14:10	Transient liquid phase bonding of γ -TiAl alloys — Understanding of microstructure development and mechanical strength with in-situ HEXRD measurements	Katja Hauschildt	HZG, Inst. of Materials Research
14:30 Coffee break			
Session 2: Imaging			
15:00	Imaging instruments at IBL, HEMS and MINAXS beamlines	Christina Krywka	<i>Chair: C. Krywka</i> HZG, Inst. of Materials Research
15:15	Loss of spatial organisation in articular cartilage during osteoarthritis - a new physiopathological model illustrated by 3d imaging	Ulf K. Hoffmann	Univ. Tübingen, Universitätsklinikum
15:35	Direct observation of coupled geochemical and geomechanical impacts on chalk microstructural evolution under elevated CO ₂ pressure	Yi Yang	Univ. Copenhagen, Department of Chemistry
15:55	Comparative head anatomy and postlarval muscle development in caddisflies revealed by μ CT	Frank Friedrich	Univ. Hamburg, Department of Biology
16:15	Final discussion		

III Poster Session

III Poster Session Topics

III.1 Facility and Beamline Poster

1. PETRA III at DESY: X-ray Photons at Highest Spectral Brilliance
O.H. Seeck, W. Drube and C.G. Schroer
2. PETRA IV
C.G. Schroer
3. FLASH
S. Toleikis for the FLASH team
4. The Swedish beamline at the PETRA III extension: side station
M. v. Zimmermann, R. Nowak, S. Sonntag and O. Gutowski
5. Status of the European Cluster of Advanced Laser Light Sources (EUCALL)
G.A. Appleby, T. Tschentscher and C. Miron
6. P03: X-ray nanodiffraction for material science
A. Davydok and C. Krywka
7. P11 at PETRA III: A versatile beamline for X-ray crystallography
A. Burkhardt, S. Panneerselvam, O. Lorbeer, J. Meyer, B. Reime, T. Pakendorf, P. Fischer, N. Stuebe, M. Warmer and A. Meents
8. European XFEL user laboratories and sample delivery support
C. Deiter, K. Dörner, R. Graceffa, M. Kitel, K. Lorenzen, J. Moore, J. Bielecki and J. Schulz
9. The Swedish Beamline at the PETRA III Extension: in-line branch
U. Lienert, S. Gutschmidt, S. Haas and T. Bäcker
10. Possibilities at the Resonant Scattering and Diffraction Beamline P09 at PETRA III
J. Stremper, S. Francoual, J.R.L. Mardegan, L.S.I. Veiga and D. Reuther
11. The high resolution diffraction beamline P08
F. Bertram, R. Kirchhof, K. Perumal, D. Hass, G. Bussone, O. Gutowski, A. Sarma, A.-C. Dippel, O. Seeck and U. Ruett
12. Russian-German Nanodiffraction Beamline at PETRA III Extension
D.V. Novikov, R. Grifone, J. Raabe and E.Kh. Mukhamedzhanov
13. Simultaneous XRF/Ptychographic Imaging using a Maia and Eiger Detector at P06 PETRA III
J. Garrevoet, A. Schropp, U. Boesenberg, D. Brückner, J. Reinhardt, R. Kirkham, S. Kalirai, F. Meirer, C.G. Schroer and G. Falkenberg
14. Inelastic x-ray scattering at the Dynamics Beamline P01 - PETRA III
H. Yavas, H. Gretarsson, M. Harder, G. Spiekermann, D. Ketenoglu, F.-U. Dill, S. Mayer, I. Sergeev and H.-C. Wille
15. Status of the EMBL BioSAXS beamline P12 at PETRA III
M.A. Schroer, C.E. Blanchet, A. Gruzinov, A. Spilotros, D.C.F. Wieland, C.M. Jeffries, M.A. Gräwert, D. Franke, N. Hajizadeh, S. Fiedler and D.I. Svergun
16. P03: in Situ and in Operando Studies of Advanced and Functional Materials
S.V. Roth, J. Rubeck, W. Ohm, M. Schwarzkopf, B. Beyersdorff and P. Pandit
17. P13/P14 - EMBL beamlines for macromolecular crystallography on PETRA III
T.R. Schneider, G. Bourenkove, G. Pompidor, I. Bento, J. Kallio, I. Karpics, A. Polyakova and S. Fiedler
18. Next generation detectors at PETRA III and FLASH - get all that data stored and analyzed
M. Gasthuber, S. Dietrich, U. Ensslin, M. Kuhn, J. Malka, T. Kracht and A. Rothkirch

19. FXE Instrument: Femtosecond X-ray Experiments at European XFEL
C. Bressler, W. Gawelda, A. Galler, D. Khakhulin, S. Schulz, F. Lima, P. Zalden, M. Knoll, P. Frankenberger and T. Korsch
20. Status of the High Resolution Powder Diffraction Beamline P02.1 at PETRA III, DESY
M. Etter, J. Bednarcik, A. Berghäuser, A. Ehnes, H.-P. Liermann, A. Schökel, I. Schwark, O. Seeck, M. Wendt and S. Wenz
21. P22 Hard X-ray (micro-) photoelectron spectroscopy
A. Gloskovskij, S. Piec, I. Sarkar, K. Ederer, I. Schostak, W. Drube, C. Wiemann, C.M. Schneider, M. Sing and R. Claessen
22. Status of the Extreme Conditions Beamline (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
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H.P. Liermann, K. Glazyrin, A. Pakhomova, E. Bykova, M. Bykov, M. Wendt, S. Wenz, A. Ehnes, I. Schwark and J.T. Roehr
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J. Buck, G. Hartmann, F. Scholz, J. Seltmann and J. Viefhaus
25. P65, the first year of user operation
E. Welter, R. Chernikov and M. Herrmann
26. DESY NanoLab
H. Noei, V. Vonk, T.F. Keller, R. Roehlsberger and A. Stierle
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U. Ruett, O. Gutowski, R. Kirchhof, F. Bertram and A.-C. Dippel
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M. Sprung, A. Ricci, E. Stellamanns, M. Kampmann, E. Schroeder and D. Weschke
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A. Kotlov, I. Schostak, W. Drube and M. Rübhausen
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M. Herlitschke, I. Sergueev, P. Alexeev, F.-U. Dill, K. Schlage, C. Strohm, O. Leupold and H.-C. Wille
32. Construction Status of the new Crystallography Beamline P24 at PETRA III
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33. CSSB - Centre for Structural Systems Biology
M. Wilmanns

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M. Osterhoff, C. Eberl, J. Soltau and H.U. Krebs
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H. Fleckenstein, M. Domaracky, T. Delmas, L. Gumprecht, S. Imlau, J. Maracke, M. Prasciolu, M. Schust, P. Talkovski, H. Chapman and S. Bajt

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36. X-ray Beam Diagnostic Imagers for the European XFEL: Progress on Installation and Commissioning
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T. Burian, J. Krzywinski, A. Andrejczuk, R.M. Bionta, V. Hajkova, L. Vysin, P. Bohacek, J. Chalupsky, M. Jurek, M. Kirm, V. Nagirnyi, S. Vielhauer, R. Sobierajski, K. Tiedtke, S. Toleikis, C. Özkan, H. Sinn, J. Gaudin, S. Bajt, H.N. Chapman, R.A. Loch, S. Moeller, K. Saskl, P. Sovak and L. Juha
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39. Temporal characterization on FLASH FEL pulses: Terahertz field driven streaking
R. Ivanov, S. Düsterer, M. Brachmanski, G. Brenner and J. Xiu
40. Probing the minimal nanowire volume by X-ray diffraction for in-situ MBE nanowire growth
J. Vogel, P. Schroth, S.M.M. Kashani, L. Feigl, J. Jakob, A. Al Hassan, A. Davtyan and U. Pietsch
41. LUX - towards laser-driven soft X-ray user beamline
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M. Lyubomirskiy, I. Snigireva and A. Snigirev
43. Scanning Coherent X-Ray Microscopy with High Spatial Resolution at Beamline P06
A. Schropp, D. Brückner, R. Döhrmann, G. Falkenberg, J. Garrevoet, M. Kahnt, J. Reinhardt, M. Scholz, M. Seyrich, J. Patommel, D. Samberg, F. Seiboth, F. Wittwer and C. Schroer
44. Efficient sub-25 nm Focusing of 12.7 keV X-rays with a Long Working Distance using Multilayer Laue Lenses
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56. KB mirror focusing optics at SPB/SFX
R. Bean
57. Laser Beam Delivery and Timing Diagnostic for the SQS Scientific Instrument
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58. Microchip Characterization at a Synchrotron
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63. Applications of X-ray streak detectors for spectroscopy, characterization, and diagnostics at SASE Free-Electron Lasers
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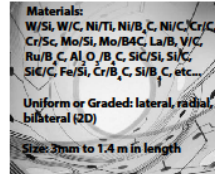


Figure 1: RIT produces multilayer coatings from a wide variety of material systems. Each material bi-layer is chosen to address a specific performance criteria such as absorption edges and energy range.

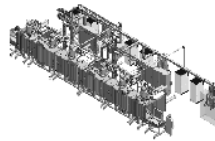


Figure 2: RIT's newest deposition system has the ability to coat a 750mm diameter or 2.1m long optic, using standard and reactive sputtering capabilities.



MULTILAYER OPTICS AND CAPABILITIES

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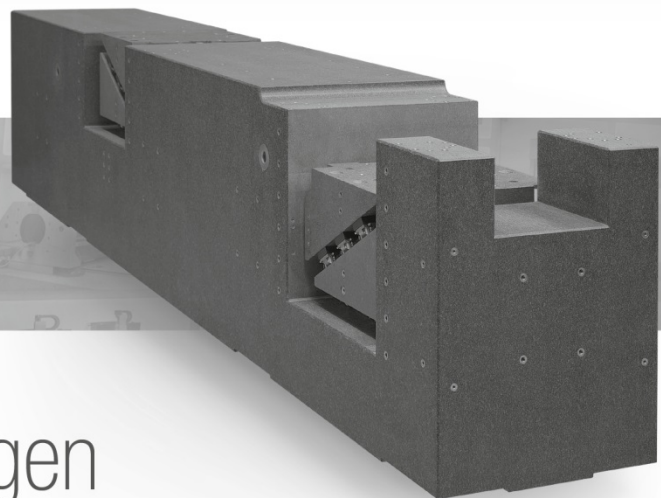
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209. Quantitative Water Window Ptychography of Cryo Fixated Bacteria
M. Rose, D. Dzbigaev, P. Skopintsev, S. Lazarev, I. Zaluzhnyy, T. Senkbeil, A. von Gundlach, S. Stuhr, C. Rumancev, Sergey Pikuz, L. Loetgering, J. Viefhaus, A. Rosenhahn and I. Vartanyants
210. Developments on liquid sample delivery at European XFEL
R. Graceffa, D. Ropers, V. Ingua, B. Perot, O. Bilsel, K. Dörner, S. Kathuria and J. Schulz
211. Dragonfly: Software for performing Single Particle Imaging structure reconstruction using the Expand-Maximize-Compress (EMC) algorithm
K. Ayyer, N.-T.D. Loh, T.Y. Lan, V. Elser and H.N. Chapman
212. Indirect selection of protein crystal containing cells using fluorescence-activated cell scanning (FACS)
W. Riekehr, R. Schönherr, J. Frenz, T. Vollbrandt and L. Redecke



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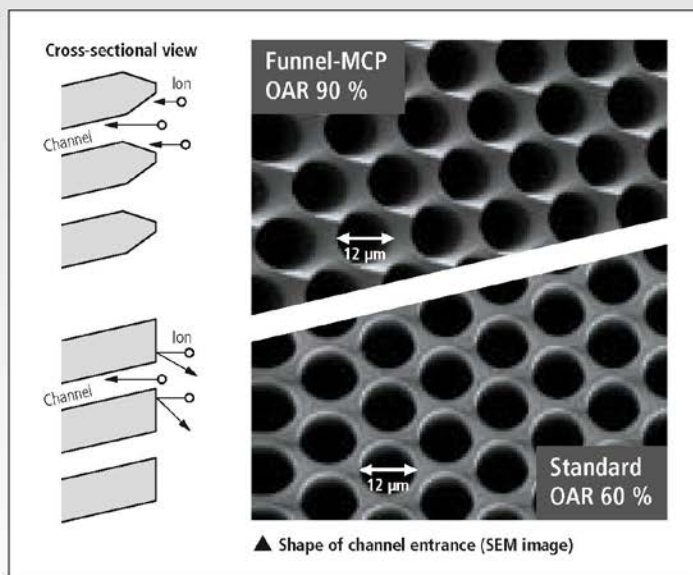
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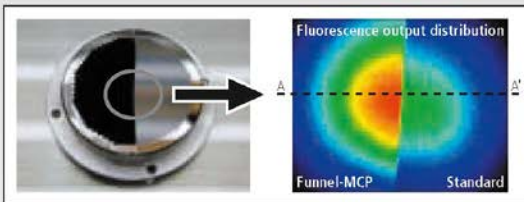
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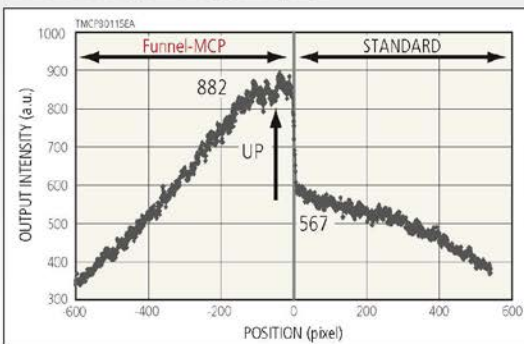
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Example of ion detection



Fluorescence output intensity profile (A-A')



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R. Schönherr, M. Rudolph, P. König, G. Hüttmann and L. Redecke
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O.M. Yefanov, K. Ayyer, A. Morgan, D. Obertuer, A. Barty and H.N. Chapman
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216. SASBDB: curated repository for biological small angle scattering data and models
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217. Ionization and fragmentation of gas-phase biomolecules
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M. Fayyaz, M. Perbandt, C. Betzel and H. Rohde
219. Reliably distinguishing protein nanocrystals from amorphous precipitate by means of depolarized dynamic light scattering
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220. Novel in situ dynamic light scattering techniques to follow the nucleation process during crystal growth
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228. Structure and strain of epitaxial ultrathin nickel ferrite films on MgO(001) and SrTiO₃(001)
T. Nordmann, J. Rodewald, O. Kuschel, K. Ruwisch, J. Thien, F. Bertram and J. Wollschläger
229. Probing ultrafast changes to a vertical spin density profile with resonant XUV magnetic reflectivity at the free-electron laser FERMI.
B. Pervaz, T. Sant, D. Keszov, F. Capotondi, E. Pedersoli, M. Kiskinova, M. Klaeui, H. Zabel, U. Pietsch and C. Gutt

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291. Structure and Dynamics in suspensions of interacting colloids studied by intensity correlation methods
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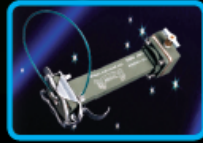
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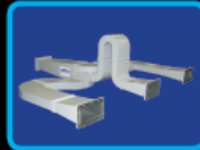
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297. Texture and defect density evolution of Mg-ZN202 during high temperature deformation by in-situ synchrotron diffraction
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298. Theory of X-ray scattering from laser-driven crystals
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301. Alloying influence on the activity of deformation and recrystallization mechanisms on the microstructure and texture development of rolled Mg-RE sheets
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324. Theoretical modeling of high energy resolution XANES of superparamagnetic iron oxide nanoparticles for theranostics in oncology
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325. Toxicity study and spectroscopy characteristic of potassium gadolinium tungstate nanocrystals
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326. Real time investigation of optical properties and morphology during the co-sputter deposition of Au/Ag nanoparticles
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328. Pump-Probe Holographic Imaging of Nanoscale Magnetic Domains
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330. Arrays of magnetic Nanodots studied by X-ray holographic Microscopy and Scattering
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VENDOR EXHIBITION

27 Jan. 2016

13.00- 18.00

Experimentierhalle 1 (Bldg. 26)

- 1 AXILON AG
- 2 PI miCos
- 3 Rigaku Innovative Technologies Inc.
- 4 SmarAct GmbH
- 5 Föhrenbach GmbH
- 6 FMB Berlin
- 7 PREVAC sp. z o.o.
- 8 BEST Fluidsysteme GmbH
- 9 bc-technology GmbH
- 10 Cryoandmore Budzylek GbR
- 11 Huber Diffraktionstechnik GmbH
- 12 GLOBES Elektronik GmbH
- 13 Pilz-Optics
- 14 Newport Spectra Physics
- 15 PINK GmbH Vakuumtechnik
- 16 Standa Ltd.
- 17 Allectra GmbH
- 18 Leybold GmbH
- 19 DECTRIS AG
- 20 + 21 Hamamatsu Photonics Deutschland
- 22 mechOnics ag
- 23 Edwards ltd
- 24 Goodfellow Gmbg
- 25 Agilent Technologies
- 26 Johann Fischer Aschaffenburg Präzisionswerk GmbH
- 27 eltherm GmbH
- 28 HORIBA Jobin Yvon GmbH
- 29 Hositrad Holland B.V.
- 30 Steinmeyer Mechatronik GmbH
- 31 Spetec GmbH
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- 33 Carl Zeiss SMT GmbH
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- 35 VACOM Vakuum Komponenten
- 36 + 37 VAT Deutschland GmbH
- 38 vaqtec-scientific
- 39 Linear- und Handhabungstechnik GmbH
- 40 Oelze GmbH
- 41 Reuter Technologie GmbH
- 42 Incoatec GmbH
- 43 Kurt J. Lesker Company
- 44 Rohde & Schwarz
- 45 LIOP-TEC GmbH
- 46 greateyes GmbH

European XFEL Users Meeting 2017

DESY Photon Science Users Meeting 2017

Vendor Exhibition Booths

27 January 2017, 13.00h -18.00h

Halle I, Bldg. 26

