DESY Photon Science Users' Meeting 2024
European XFEL Users' Meeting 2024

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

DESY Photon Science Users' Meeting 2024
European XFEL Users' Meeting 2024
in Hamburg, Germany
Main venue: "Kuppel Hamburg"

(Dome on the Trabrennbahn Bahrenfeld opposite to the DESY campus (side gate), Luruper Chaussee 30)

DRAFT Programme!

Monday, January 22: Satellite Workshops

		Organiser or Affiliation
09:00	Grazing-incidence X-ray experiments using FELs	European XFEL
14:00	Seminar: Plasma Undulator and Plasma Wakefield Acceleration with Externally Injected and Self-injected e-Beams	European XFEL
13:00	Status and research highlights of the ECB (P02.2) at PETRA III	DESY
12:30	Momentum microscopy at PETRA and FLASH	DESY

Tuesday, January 23: Satellite Workshops

09:00	Molecular Water Science	European XFEL
09:00	Eurizon 2020+ workshop on FEL linac driver and FEL physics applications	European XFEL
13:00	Status of the HED instrument and the HIBEF contributions as well as scientific highlights	European XFEL
09:00	Community proposals using seeded operation at FLASH	DESY
13:00	Opportunities for ultrafast electron diffraction (UED) experiments at DESY's REGAE facility	DESY
13:00	News from Computing for Photon Science	DESY
13:00	In situ energy-dispersive XRD and imaging on materials in the Large Volume Press at P61B	DESY

Wednesday, January 24: European XFEL Users' Meeting & Satellite Workshops

09:00	High Energy X-ray Diffraction for Physics and Chemistry	DESY
10:00	SAXS/ WAXS/ GISAXS @ DESY	DESY
13:30	14th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III	DESY
13:00	ROCK-IT Outreach Meeting & Workshop	DESY
14:00	Analytics for Battery Technologies & Recycling	DESY
12:00	The Swedish Materials Science beamline at PETRA III	DESY

08:30 - 10:00	**Registration**		
10:00 - 10:20	**Opening Session**		
10:00	Welcome	Thomas Feurer	*European XFEL*
10:10	Opening address from the Council Chair	Federico Boscherini	*University Bologna*
10:15 - 12:30	**European XFEL Update Session**		*Chairperson: Sakura Pascarelli (European XFEL)*
10:15	General status of the project	Thomas Feurer	*European XFEL*
10:45	Accelerator and FEL sources: status and future plans	Shan Liu	*DESY*
11:15	Characterization and applications of attosecond X-ray pulses	Michel Meyer	*European XFEL*
11:45	News from the European XFEL User Organization and Bestowal of the Young Scientist Award	Marc Simon	*Sorbonne University, France*
12:00	Young Scientist talk	To be announced	
12:30 - 14:00	**Lunch break**		
14:00 - 15:30	**Science Session I**		*Chairperson: Kartik Ayyer (MPSD)*
14:00	Ultrafast X-ray spectroscopy of photochemical bond activation reactions	Raphael Jay	*Uppsala University, Sweden*
14:30	Non-equilibrium shape variations amongst millions of nanoparticles	Duane Loh	*National University of Singapore*

15:00	Experimental Foundations for Exploring Crystallographic 'Dark Matter'	James Hohman	*University Connecticut, US*
15:30 - 16:00	**Coffee break**		
16:00 - 17:30	**Science Session II**		*Chairperson: Serguei Molodtsov (European XFEL)*
16:00	Low-Z Mixtures at Planetary Interior Conditions	Alessandra Ravasio	*LULI, France*
16:30	Imaging soft X-ray spectroscopy at SQS: a side view on non-linear processes	Jan-Erik Rubensson	*Uppsala University, Sweden*
17:00	Imaging via photon-photon correlation of X-ray fluorescence	Fabian Trost	*DESY/CFEL European XFEL*
17:30-20:00	**POSTER SESSION I and Vendor exhibition (14h)**		**Coffee break**
until 21:30	**European XFEL Get Together**		**Light dinner**

Thursday, 25 January: Soft X-ray FEL Science Highlights (jointly organ.) & Satellite Workshops

09:00	XAFS at P64/65 and perspectives for future PETRA III and IV beamlines		DESY
09:30	Introduction to PYDIDAS: A new tool for automated diffraction data analysis		Hereon
12:50	Helmholtz-Zentrum Hereon GEMS Outstation: Materials Research and High Resolution Imaging		Hereon
08:30	**Registration**		
			Chairperson: Marc Simon (Sorbonne Univ.)
09:00	Probing molecular dynamics of uracil by time-resolved X-ray photoelectron spectroscopy	Oksana Plekan	*Elettra - Sincrotrone Trieste, Italy*
09:30	Photo-excited dynamics of an electron-doped cuprate via tr-RIXS	Wei-Sheng Lee	*Stanford University, US*
10:00	Real-time observation of non-equilibrium phonon-electron energy flow in laser-heated nickel	Vishal Shokeen	*Uppsala University, Sweden*
10:30	FERMI update - status and perspectives	Claudio Masciovecchio	*Elettra - Sincrotrone Trieste, Italy*
11:00 - 11:30	**Coffee break**		

DESY Photon Science Users' Meeting

			Chairperson: Rolf Treusch (DESY)
11:30	Welcome to the FEL Session	Franz Kärtner	*DESY/Univ. Hamburg*
11:35	FLASH status und strategy	Markus Gühr	*DESY Hamburg*
12:15	FLASH 2020+ Activties - Update	Lucas Schaper	*DESY Hamburg*
12.35 - 14.00	**Lunch break**		
			Chairperson: Kai Tiedtke (DESY)
14:00	Fifty shades of silver: femtosecond snapshots of plasmonic nanoparticles and their ultrafast melting	Alessandro Colombo	*ETH Zürich, Switzerland*
14:30	FLASH FEL pump-probe laser concept based on spectral broadening of high-power ytterbium picosecond systems in multi-pass cells	Anne-Lise Viotti	*Lund University, Sweden*
15:00	Time-Resolved X-ray Photoelectron Spectroscopy: Ultrafast Dynamics in CS2 Probed at the S 2p Edge	Ian Gabalski	*SLAC, Stanford, US*
15:30	*The European Synchrotron and FEL User Organisation (ESUO): Advocating for European users*	Bridget Murphy (ESUO vice president)	*CAU Kiel*
16:00-19:00	**POSTER SESSION II and Vendor exhibition (14h)**		**Coffee break**
until 21:30	**DESY Get Together**		**Light dinner**

Friday, January 26: DESY Photon Science Users' Meeting & Satellite Meetings

09:00	Data management, analysis, and reduction at European XFEL		European XFEL
08:30	**Registration**		

		Chairperson: Franz Kärtner (DESY)	
09:00	Welcome and Future DESY	Helmut Dosch	*DESY Hamburg*
09:20	Overview DESY Photon Science 2023	Edgar Weckert	*DESY Hamburg*
09:55	PETRA IV	Harald Reichert	*DESY Hamburg*
10:25 - 11:00	**C o f f e e b r e a k**		
		Chairperson: Hans-Christian Wille (DESY)	
11:00	PETRA III Status	Christian Schroer	*DESY/Univ. Hamburg*
11:40	Investigating biomolecular structure in the aqueous phase using photoemission spectroscopy	Bernd Winter	*FHI MPG Berlin, Germany*
12:10	The iron spin crossover in ferropericlase at high temperatures: implications for seismic observations	Viktoria Trautner	*University of Oxford, UK*
12:40	Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5′-monophosphate decarboxylase catalysis	Kai Tittmann	*Georg-August Univ. Göttingen, Germany*
13:10	Report of the 'DESY Photon Science User Committee' (DPS-UC)	Peter Müller-Buschbaum (DPS-UC Chair)	*TU München, Germany*
13:25	DESY Photon Science User Award 2023 ceremony	Heinz Graafsma (Chair Award commit.)	*DESY*
13:30	Research with Photons – Light for the Future: News from the KFS (Committee Research with Synchrotron Radiation)	Christian Gutt (KFS Chair)	*Univ. Siegen, Germany*
13.45			

Overview Satellite Meetings

Monday, 22. January 2024

European XFEL | **Grazing-incidence X-ray experiments using FELs**
Start time: 09.00h | European XFEL | XHQ building, room E1.173

European XFEL | **Seminar: Plasma Undulator and Plasma Wakefield Acceleration with Externally Injected and Self-injected e-Beams**
Start time: 14:00h, Location: DESY, Seminar room 4a/b, Bldg. 1b, 2.floor

DESY | **Status and research high-lights of the ECB (P02.2) at PETRA III**
Start time: 13.00h | FLASH Seminar room, Bldg. 28c

DESY | **Momentum microscopy at PETRA and FLASH**
Start time: 12.30h | CSSB auditorium, Bldg. 15

Tuesday, 23 January 2024

European XFEL | **Molecular Water Science**
Start time: 9:00h | European XFEL | XHQ building, room E1.173

European XFEL | **Eurizon 2020+ workshop on FEL linac driver and FEL physics applications**
Start time: 09:00h | European XFEL | XHO building, Think Tank room

European XFEL | **Status of the HED instrument and the HIBEF contributions as well as scientific highlights**
Start time: 13:00h | European XFEL | XHO building, Lounge

DESY | **Community proposals using seeded operation at FLASH**
Start time: 09:00h | Seminar room CFEL I-III, Bldg. 99

DESY | **Opportunities for ultrafast electron diffraction (UED) experiments at DESY's REGAE facility**
Start time: 13:00h | FLASH Seminar room, Bldg. 28c

DESY | **News from Computing for Photon Science**
Start time: 13:00h | CSSB auditorium, Bldg. 15

DESY | **In situ energy-dispersive XRD and imaging on materials in the Large Volume Press at P61B**
Start time: 13:00h | Seminar room BAH 1+2, Bldg. 3

Wednesday, 24 January 2024

DESY | **High Energy X-ray Diffraction for Physics and Chemistry**
Start time: 09:00h | CSSB auditorium, Bldg. 15

DESY | **SAXS/ WAXS/ GISAXS @ DESY**
Start time: 10:00h | DESY Auditorium, Bldg. 5

DESY | **14th Workshop on X-Ray Nano-Imag-ing of Biological and Chemical Systems at PETRA III**
Start time: 13:30h | FLASH Seminar room, Bldg. 28c

DESY | **ROCK-IT Outreach Meeting & Workshop**
Start time: 13:00h | DESY, Seminar room 4a/b, Bldg. 1b, 2.floor

DESY | **Analytics for Battery Technologies & Recycling**
Start time: 14:00h | DESY, Seminar room CFEL II-III, Bldg. 99

DESY | **The Swedish Materials Science beamline at PETRA III**
Start time: 12:00h | DESY, Seminar room 109, Bldg. 25b

Thursday, 25 January 2024

DESY | **XAFS at P64/65 and perspectives for future PETRA III and IV beamlines**
Start time: 09:00h | FLASH Seminar room, Bldg. 28c

Hereon | **Introduction to PYDIDAS: A new tool for automated diffraction data analysis**
Start time: 09:30h | Seminar room CFEL I-III, Bldg. 99

Hereon | **Helmholtz-Zentrum Hereon GEMS Outstation: Materials Research and High Resolution Imaging**
Start time: 12:50h | Seminar room CFEL I-III, Bldg. 99

Friday, 26 January 2024

European XFEL | **Data management, analysis, and reduction at European XFEL**
Start time: 09:00h via Zoom

General Information

Main sessions and poster sessions
All these sessions will take place in the dome “Kuppel Hamburg”.

The “Kuppel Hamburg” is located on the “Trabrennbahn Bahrenfeld”, outside of the DESY campus opposite the side gate. Address: Luruper Chaussee 30, 22761 Hamburg (see map).

Vendor exhibition
The vendor exhibition will take place in the “Kuppel Hamburg” on Wednesday (25 Jan.) and Thursday (26 Jan.) 14:00-20:00

Satellite meetings and workshops
All satellite meetings and workshops will take place in seminar rooms on the DESY or European XFEL campus as indicated in this programme.

Get together (at the “Kuppel Hamburg”)
European XFEL Users’ Meeting - Wednesday, 24 January, starting 19:30
DESY Photon Science Users’ Meeting - Thursday, 25 January, starting 19:30

Free WLAN (eduroam, Science-Hotspot etc.) is available on the DESY or European XFEL campus, but not in the “Kuppel Hamburg”!

Organisers
K. Baranašić (European XFEL), S. Bertini (European XFEL), G. Heeßel (European XFEL), T. Kobaidze (European XFEL), M. Kreuzeder (DESY), K. Kucza (DESY), W. Laasch (DESY), F. Lehmkühler (DESY), S. Pascarelli (European XFEL), G. Quondam (European XFEL), A. Rodriguez-Fernandez (European XFEL), A. Rothkirch (DESY), D. Unger (DESY)

Local Information

Meals
Breakfast
If you stay at the DESY guest house you may have breakfast in the DESY canteen (opens at 07:00, Bldg. 9) or CFEL Cafeteria (opens at 8:00, Bldg. 99) at your own expenses. If you stay at the European XFEL Guest House you may have breakfast at BeamStop restaurant (07:00-10:00) at your own expenses.

Lunch
Please note that due to the refurbishment of the DESY canteen, lunch will be available in the “Kuppel Hamburg” on Wednesday and Thursday during the lunch breaks of the main sessions. The service in the DESY canteen is organised slightly differently and partly in a tent in front of the canteen. However, you may also have lunch or snacks n the DESY canteen (Bldg. 9; 11.00 to 14.00) or CFEL Cafeteria (Bldg. 99; 8:00-15:00) at your own expenses. Please try to avoid the queues during the main opening hours. At the European XFEL campus in BeamStop restaurant lunch service is available from 11:30-14:00, coffee service is available from 07:00-15:00, at your own expenses.

Public Transportation
Bus (HVV): Bus stops near the “Kuppel Hamburg” and the side entrance: ‘Luruper Chaussee (DESY)’ or the main entrance: “Trabrennbahn Bahrenfeld”. (Exclusively *Cashless payment in buses since 2024, but only via HVV app, prepaid HVV card or pre-purchased ticket*). Further information: www.hvv.de
Bike rental (StadtRAD Hamburg): Two city bike stations are on the DESY campus where bikes can be returned. Further information: stadtrad.hamburg.de


DESY
Campus in Hamburg-Bahrenfeld
Location Users' meeting
'Kuppel Hamburg'
Luruper Chaussee 30
22761 Hamburg
Side gate
Main gate
DESY guest house
Luruper Chaussee/DESY
Bus 2, 3, X3, 284
Trabrennbahn
Bahrenfeld
Luruper Chaussee
Notkestraße
Ebertallee
Hamburg City
Bertr.-Russel-Straße
Albert-
Einstein-
Ring
Max-Born-Straße
European XFEL
CSSB
Footpath to Footpath to Users'meeting
(Trabrennbahn)


SRI2024
15th International Conference on
Synchrotron Radiation Instrumentation
26-30 August 2024 • Hamburg, Germany
Registration opens February 2024
Further information: www.sri2024.eu

I Main sessions
Abstracts of the talks

Ultrafast X-ray spectroscopy of photochemical bond activation reactions

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4d and 5d metal carbonyls are widely recognized for their photochemical C-H bond activation capabilities. UV excitation of these complexes leads to CO dissociation and the formation of a reactive metal center, which rapidly binds alkane C-H groups from solution and ultimately breaks the C-H bond [1]. The reactivity of 3d metal carbonyls following photoinduced CO dissociation, however, is often hampered by the formation of triplet species, which instead are reactive towards Si-H bond activation [2]. We have used ultrafast X-ray absorption spectroscopy and resonant inelastic X-ray scattering at the transition metal L-edge to access and evaluate the valence electronic structure locally at the reactive metal center [3,4]. We follow the photochemical bond activation pathway of a Rhodium and a Cobalt carbonyl complex all the way from the initial femtosecond excited-state and dissociation dynamics to pico-to-nanosecond bond activation. We find previously undetected transient reaction intermediates and characterize how their electronic structure dictates their varying reactivity and catalytic function on ultrafast timescales. We experimentally access, to the best of our knowledge for the first time, the essential charge-transfer orbital interactions, which make metal carbonyls reactive and which determine how they bind and break incoming C-H or Si-H bonds.

References

[1] R. G. Bergmann, C-H activation**,** Nature **446**, 391-393 (2007)

[2] P. T. Snee et al., Triplet Organometallic Reactivity under Ambient Conditions: An Ultrafast UV Pump/IR Probe Study, Journal of the American Chemical Society **123**, 2255-2264, (2001)

[3] R. M. Jay et al., Tracking C–H activation with orbital resolution, Science **380**, 955-960, (2023)

[4] A. Banerjee et al., Accessing Metal-Specific Orbital Interactions in C-H Activation with Resonant Inelastic X-ray Scattering, Chemical Science, (2024), https://doi.org/10.1039/D3SC04388F

Non-equilibrium shape variations amongst millions of nanoparticles

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Nanoparticles, exhibiting functionally relevant structural heterogeneity, are at the forefront of cutting-edge research. High-throughput single-particle imaging (SPI) with x-ray free-electron lasers (XFELs) creates unprecedented opportunities for recovering the shape distributions of millions of particles that exhibit functionally relevant structural heterogeneity. To realize this potential, three challenges have to be overcome: (1) simultaneous parametrization of structural variability in real and reciprocal spaces; (2) efficiently inferring the latent parameters of each SPI measurement; (3) scaling up comparisons between 10^5 structural models and 10^6 XFEL-SPI measurements.

Here, we describe how we overcame these three challenges to resolve the non-equilibrium shape distributions within millions of gold nanoparticles imaged at the European XFEL.

These shape distributions allowed us to quantify the degree of asymmetry in these particles, discover a relatively stable shape envelope amongst nanoparticles, discern finite-size effects related to shape-controlling surfactants, and extrapolate nanoparticles' shapes to their idealized thermodynamic limit.

Ultimately, these demonstrations show that XFEL SPI can help transform nanoparticle shape characterization from anecdotally interesting to statistically meaningful.

Experimental Foundations for Exploring Crystallographic ‘Dark Matter’

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Single crystal X-ray diffraction provides structural models for a growing number of new materials each year. However, solved structures are biased towards those that are easily crystallized. Hybrid materials, those compounds that contain both inorganic and organic components, often yield crystals too small or otherwise pathological to be used for traditional characterization techniques. These are the “dark” materials that are either too difficult or too time-consuming to characterize, and they make up a large portion of hypothetical hybrid materials. We have applied a technique of small-molecule serial femtosecond chemical crystallography (smSFX) that uses the high brightness of an X-ray free-electron laser to acquire diffraction from crystals in the 1-5 micron range.[1-3] Graph theory is used to index those snapshots, enabling the determination of crystal structure by solving the instantaneous rotational matrix of the crystals in the path of the XFEL beam. We used this technique to explore the ligand environment with variables of steric hindrance, functional group, and intermolecular forces, each addressed by selecting different ligand shapes and configurations. We find dramatic differences in the connectivity, topology, and dimensionality of the resulting silver organothiolates. Of note is the nature of the Ag-Ag interactions, which appear to be an important component of the fine structure of the silver systems. The Ag-Ag networks are found to rearrange as a function of the supramolecular ordering of each example system. Examples of solved XFEL structures will be presented and the outlook for smSFX as a crystallography technique will be considered.

References

[1] Aleksich, M.; Paley, D. W.; Schriber, E. A.; Linthicum, W.; Oklejas, V.; Mittan-Moreau, D. W.; Kelly, R. P.; Kotei, P. A.; Ghodsi, A.; Sierra, R. G.; Aquila, A.; Poitevin, F.; Blaschke, J. P.; Vakili, M.; Milne, C. J.; Dall’Antonia, F.; Khakhulin, D.; Ardana-Lamas, F.; Lima, F.; Valerio, J.; Han, H.; Gallo, T.; Yousef, H.; Turkot, O.; Bermudez Macias, I. J.; Kluyver, T.; Schmidt, P.; Gelisio, L.; Round, A. R.; Jiang, Y.; Vinci, D.; Uemura, Y.; Kloos, M.; Hunter, M.; Mancuso, A. P.; Huey, B. D.; Parent, L. R.; Sauter, N. K.; Brewster, A. S.; Hohman, J. N., Xfel Microcrystallography of Self-Assembling Silver N-Alkanethiolates. *J. Am. Chem. Soc.* **2023,** *145*, 17042-17055. 10.1021/jacs.3c02183

[2] Schriber, E. A.; Paley, D. W.; Bolotovsky, R.; Rosenberg, D. J.; Sierra, R. G.; Aquila, A.; Mendez, D.; Poitevin, F.; Blaschke, J. P.; Bhowmick, A.; Kelly, R. P.; Hunter, M.; Hayes, B.; Popple, D. C.; Yeung, M.; Pareja-Rivera, C.; Lisova, S.; Tono, K.; Sugahara, M.; Owada, S.; Kuykendall, T.; Yao, K.; Schuck, P. J.; Solis-Ibarra, D.; Sauter, N. K.; Brewster, A. S.; Hohman, J. N., Chemical Crystallography by Serial Femtosecond X-Ray Diffraction. *Nature* **2022,** *601*, 360-365. 10.1038/s41586-021-04218-3

[3] Kotei, P. A.; Paley, D. W.; Oklejas, V.; Mittan-Moreau, D. W.; Schriber, E. A.; Aleksich, M.; Willson, M. C.; Inoue, I.; Owada, S.; Tono, K.; Sugahara, M.; Inaba-Inoue, S.; Aquila, A.; Poitevin, F.; Blaschke, J. P.; Lisova, S.; Hunter, M. S.; Sierra, R. G.; Gascón, J. A.; Sauter, N. K.; Brewster, A. S.; Hohman, J. N., Engineering Supramolecular Hybrid Architectures with Directional Organofluorine Bonds. *Small Science n/a*, 2300110. https://doi.org/10.1002/smsc.202300110

Low-Z Mixtures at Planetary Interior Conditions

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Mixtures of water, ammonia and methane are predicted to be the major components of the depths of the ice giant planets Uranus (U) and Neptune (N). The complex chemical properties that these light mixtures exhibit at high pressures (few Mbar) and temperatures (few 1000 K) crucially shape the internal structure and evolution of this class of planets and they are at the base of unresolved fundamental issues [1,2].

The physical and chemical behavior of such systems at the extreme pressures and temperatures of planetary interiors is also extremely interesting on its own, since those conditions are characterized by a coexistence of dissociated atoms, atomic clusters, chains and superionic lattices. In spite of its great appeal, exploring these phenomena is a real challenge for both *ab initio* calculations and experiments so that dedicated studies remain very limited.

Here we present our recent work combining results from experiment at various facilities (LULI, LCLS LL58 collaboration and EuXFEL 4463 collaboration) and *ab initio* simulations to investigate C-H-N-O mixtures under strong dynamic compression. In particular we will focus on the formation of so-called superionic structures, i.e., protonic conductors [3], which may help to explain the peculiar magnetic fields observed for U/N and on the diamond formation from strongly compressed C-H-N-O samples.

References

[1] R. Helled et al., Astrophysical Journal Letters 805, L11 (2015).
[2] M. Bethkenhagen et al., Astrophysical Journal 848, 67 (2017).
[3] C. Cavazzoni et al., Science 283, 44-46 (1999)

Imaging soft X-ray spectroscopy at SQS: a side view on non-linear processes

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A novel spectrometer (Fig.1), installed at the SQS instrument as a Swedish in-kind contribution to European XFEL, measures soft X-ray emission spectra (XES) spatially resolved along the path of the incident radiation.

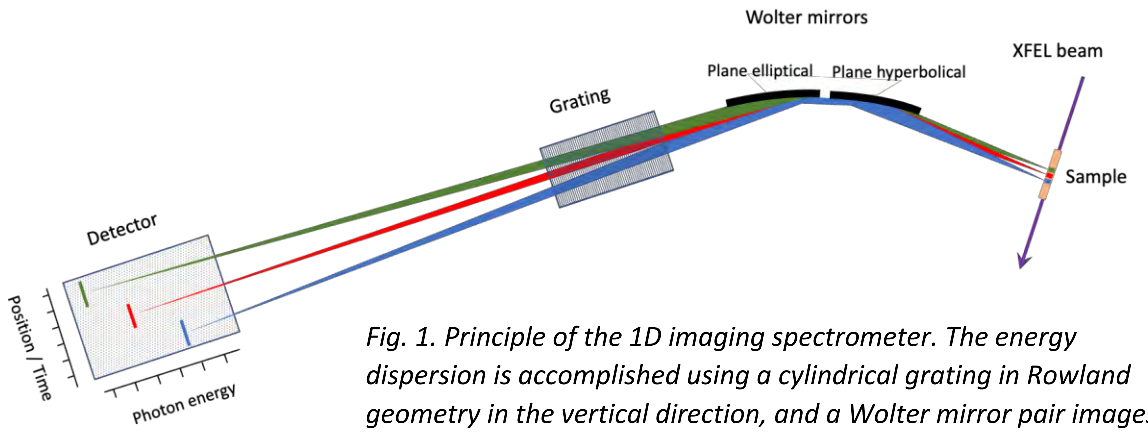

Fig. 1. Principle of the 1D imaging spectrometer. The energy dispersion is accomplished using a cylindrical grating in Rowland geometry in the vertical direction, and a Wolter mirror pair images the interaction region on the detector with ten times magnification in the horizontal plane.

The spatial resolution is used to investigate the non-linear interaction between X-rays and matter, e.g., the evolution of X-ray lasing, pulse propagation in media, and plasma dynamics. In the future it will enable pump-probe experiments with jitter-free consecutive delays in combination with an optical laser.

Some first results will be presented and discussed, including:

- State-resolved X-ray emission from single and double core holes of all charge states of Ne. Population pathways comprising resonances and intriguing threshold behavior are captured via the dependence of the spectra on incident photon energy, pulse energy and target density.
- Post-pulse excitations involving long-lived core holes in He-like Ne, monitored with time-resolved XES and imaging of the propagation at various target densities
- Unusual resonant behavior of resonant inelastic scattering with SASE pulses.
- Non-linear dissociation dynamics and propagation effects in O_2, observed via XES imaging in few-fs X-ray pump-X-ray probe experiments.

The experimental results emerge from beamtimes based on two community proposals in a collaboration involving twenty-one research institutions. The data are analyzed in terms of state-of-the-art theory.

Imaging via photon-photon correlation of X-ray fluorescence

Fabian Trost[1]

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In "coherent diffraction imaging" (CDI) methods, fluorescence is seen as a disturbing background due to its incoherent nature. However, when utilizing XFEL excitation pulses that are comparable short to the coherence time of the fluorescence photon-photon correlation can be used to retrieve the density distribution of the fluorescence emitters. This method of imaging via photon-photon correlation of X-ray fluorescence is also known as "incoherent diffraction imaging" (IDI) and corresponds to the "intensity interferometry", known from astronomy.

Contrary to coherent imaging methods, in IDI higher detected numbers of photon counts do not always correspond to a larger signal-to-noise ratio (SNR). As one consequence, for example, crystallography is not a reasonable method for IDI, since the SNR will drop with each additional unit cell. It can be generalized that more complex emitter distributions are harder to image via IDI than simpler ones. [1]

An experiment was successfully be performed at MID/EuXFEL, using a simple, yet non-trivial distribution of fluorescing copper atoms to demonstrate the feasibility of IDI. Finally, we will discuss on how IDI can be utilized for focus characterization or pulse-length determination at XFELs. [2]

References

[1] Fabian Trost, Kartik Ayyer, Henry N Chapman -- Photon statistics and signal to noise ratio for incoherent diffraction imaging -- *New J. Phys.* **22** 083070 (2020)

[2] Fabian Trost *et al.* -- Imaging via Correlation of X-Ray Fluorescence Photons -- *Phys. Rev. Lett.* **130**, 173201 (2023)

Probing molecular dynamics of uracil by time-resolved X-ray photoelectron spectroscopy

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Despite the fact that the photodynamics of DNA/RNA bases has been explored extensively by various spectroscopic techniques, time-resolved studies where a UV-pulse (or pump) is used for promoting the system to a valence electronically excited state, and an X-ray pulse (probe) is used for further excitation or ionization a core electron are still rare.

In the present work, time-resolved X-ray photoemission spectroscopy (TR-XPS) at the C, N, and O K-edges was applied in order to obtain detailed information about photoinduced dynamics of the isolated nucleobase uracil. The key advantages of TR-PES with X-rays arise from the highly localized nature of core electrons which makes them particularly sensitive to their specific chemical environment [1-3].

Through TR-XPS, the distinct femtosecond to picosecond timescales associated with the internal conversion between higher (ππ*) and lower (nπ*) singlet exited states, as well as intersystem crossing to the triplet manifold of uracil, have been observed.

References

[1] F. Brausse et al. Real-time interfacial electron dynamics revealed through temporal correlations in x-ray photoelectron spectroscopy. Struct. Dyn. **8**, 044301 (2021).

[2] M. L Vidal et al. Correction: Dyson orbitals within the fc-CVS-EOM-CCSD framework: theory and application to X-ray photoelectron spectroscopy of ground and excited states. Phys. Chem. Chem. Phys. **22**, 3744 (2020).

[3] D. Mayer et al. Following excited-state chemical shifts in molecular ultrafast x-ray photoelectron spectroscopy. Nature communications **13**, 198 (2022).

Photo-excited dynamics of an electron-doped cuprate via tr-RIXS

Wei-Sheng Lee

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Investigating the ultrafast dynamics in photo-excited quantum materials is a topic of strong interest in materials science research. To date, available time-resolved probes have revealed information about the lattice, symmetry, and electronic band structure. However, the information about the collective excitations in energy-momentum space, such as magnons and plasmons, are largely unavailable due to the lack of a suitable method. The advent of high repetition rate x-ray free-electron lasers enables time-resolved resonant inelastic scattering (RIXS) experiments, which accesses elementary excitations associated with the magnetic, charge, orbital, and lattice degrees of freedom, thus providing the previously missing pieces of information. In this presentation, I will present our tr-RIXS measurement on the electron-doped cuprates $Nd_{2-x}Ce_xCuO_4$. A photoexcitation-induced, change of the paramagnon, plasmon, and orbital excitations spectrum were observed. The momentum and time dependence will be discussed.

Fifty Shades of Silver: femtosecond snapshots of plasmonic nanoparticles and their ultrafast melting

Alessandro Colombo

ETH Zürich

Imaging nanomatter in strongly out-of-equilibrium states is extremely challenging. On the one hand, high spatial resolution is required to observe details at the nanoscale. On the other hand, its unstable nature carries to fast phenomena, which require high temporal resolution to be captured. XUV and X-ray Free Electron Lasers (FELs) are a unique tool for probing matter in such conditions, thanks to the short wavelength of the delivered coherent radiation and the large amount of photons produced, condensed in pulses of femtosecond time duration. We present experimental results obtained at FLASH on silver clusters of around 100 nm size. First, their structure is determined from the light scattered up to large scattering angles with a novel imaging technique, which allows the full three-dimensional reconstruction of their spatial distribution from a single diffraction pattern. Imaging results reveal symmetric morphologies as well as architectures with structural defects, which give insights into their formation process. This structural analysis prepares the ground for the following investigation of the dynamics of the silver cluster in superheated conditions. The silver nanoparticles are efficiently heated via a 400 nm laser, resonant with their Mie plasmon frequency, reaching temperatures of thousands of kelvin in few picoseconds. Their spatial evolution over time is investigated by recording diffraction images of the FEL light at different delays from the 400 nm laser. The two-dimensional projection of the samples density is then retrieved following the Coherent Diffraction Imaging scheme. These ultrafast snapshots of the melting silver clusters unveil a plethora of phenomena, which span from the slow melting in hundreds of picoseconds to violent explosions in few tens of picoseconds. Comparisons with molecular dynamics simulations allow the investigation of thermodynamic properties of silver in regions of its phase diagram hardly accessible so far. The outcome of this pioneering experiment stimulated a second, more recent, investigation at higher spatial resolution, by employing commercially-produced silver nanocubes of 90 nm size. Preliminary analysis, aided by Machine Learning, confirms the observed phenomena and unveils high-resolution details on the role of the sample's symmetries in the ultrafast melting dynamics.

Pump-probe laser concept for FLASH based on spectral broadening of high-power ytterbium picosecond systems

Anne-Liese Viotti

Lund University

Many user experiments at the FLASH free electron laser (FEL) are pump-probe experiments that combine the extreme UV or soft x-ray light from the FEL together with ultrashort pulses from optical lasers. Thus, developing sources that provide extended wavelength tunability, shorter pulses and reduced arrival time jitter can increase the scientific opportunities and time resolution for x-ray FEL-optical laser pump-probe experiments. The laser development at FLASH progressively transitions from TI:Sapphire systems and optical parametric chirped pulse amplification towards high-power, high repetition rates Yb:YAG lasers to match the (up to) MHz intra-burst repetition rate of the soft x-ray source. The high-power Yb:YAG lasers can be used with nonlinear pulse compression stages enabled by the multi-pass cell spectral broadening technique to reach short pulse durations.

In this talk, we present preliminary studies for a novel pump-probe laser concept at FLASH, based on the post-compression of high-power Yb:YAG amplifiers. Flexible reduction of the pulse duration is facilitated by spectral broadening in pressure-tunable multi-pass cells. As an application, we show the pumping of an optical parametric amplifier with 150 fs post-compressed pulses. By means of an additional difference frequency generation stage, tunable spectral coverage from 1.3 to 16 µm is reached with multi-µJ, sub-150 fs pulses. We also report on pulse compression to 8.2 fs duration with a double-stage multi-pass cell spectral broadening unit. Finally, we mention the current characteristics of the multi-pass cell-based pump-probe laser at the FLASH plane-grating beamlines.

Acknowledgments:
FS-LA – DESY: M. Seidel, S. Alisauskas, A. Tajalli, O. Akcaalan, J. Darvill, N. Ekanayake, U. Grosse-Wortmann, C. Li, C. Mohr, F. Pressacco, N. Schirmel, A. Swiderski, H. Tavakol, H. Tünnermann, C. Vidoli, L. Winkelmann, C. M. Heyl, B. Manschwetus, H. Cankaya, I. Hartl

Time-resolved X-ray Photoelectron Spectroscopy: Ultrafast Dynamics in CS2 Probed at the S 2p Edge

Ian Gabalski

SLAC, Stanford University

Time-resolved photoelectron spectroscopy has played a pivotal role in the elucidation of ultrafast non-adiabatic dynamics in molecules. While this technique yields information about the evolving electron binding energies, photoionization cross-sections, and photoelectron angular distributions that accompany chemical rearrangement, the application of the method has historically been limited by available ultraviolet wavelengths to studies of the delocalized valence shells. Recent developments in X-ray free-electron lasers have enabled a novel site-selective probe of coupled nuclear and electronic dynamics in photoexcited molecules: time-resolved X-ray photoelectron spectroscopy (TRXPS). TRXPS is sensitive to the evolution of the inner-shell binding energy at a specific atomic site due to changes in its local bonding environment and charge density, enabling the probing of chemical dynamics from the perspective of specific atoms.

We present results from a joint experimental and theoretical TRXPS study into the well-characterized ultraviolet photodissociation of CS2, a prototypical system for understanding non-adiabatic dynamics. Gas-phase CS2 was photoexcited with 200 nm UV pulses and probed by photoionization above the sulfur 2p edge at the CAMP@FLASH end-station. The measured spectroscopic features can be partitioned into at least three distinct regions in energy, each with their own unique time dependence. We assign these features to the transient excited state and subsequent CS and S products via comparison to a first-principles determination of the TRXPS based on Ab Initio Multiple Spawning (AIMS) simulations. Our results demonstrate the use of TRXPS as a local probe of complex ultrafast photodissociation dynamics involving multimodal vibrational coupling, non-radiative transitions between electronic states, and multiple final product channels.

Investigating biomolecular structure in the aqueous phase using photoemission spectroscopy

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Liquid-jet photoemission spectroscopy enables direct probing of electronic structure in aqueous solutions, and we demonstrate the applicability of this technique to biomolecules in a complex environment. We explore site-specific information on the interaction of adenosine triphosphate (ATP(aq)) with magnesium (Mg2+(aq)) in the aqueous phase, based on the simultaneous analysis of valence, core-level, and non-local autoionization electron signals. This study provides a comprehensive view of the electronic structure of ATP(aq) as well as the Mg2+–ATP(aq) complexes relevant to phosphorylation and dephosphorylation reactions connected with the energy conversion in biochemical processes. A second application I will discuss is the ability of liquid-jet photoelectron spectroscopy to distinguish isomeric structures in aqueous phase. The focus is on the anomeric effect in sugar aqueous solution, and specifically on methylated glucose, where each anomer, methyl a- or b-glucopyranoside, is the only form present, unlike in the case of glucose. We observe a reversal of the anomeric effect as a function of protonation state upon pH variation, based on the differences in the respective valence and core-level photoelectron spectra for the two anomers at given charge state. Overall, our approach has the potential to detail the origin of the anomeric effect.

The iron spin crossover in ferropericlase at high temperatures: Implications for seismic observations

Viktoria E. Trautner

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The second most abundant mineral in Earth's lower mantle is (Mg,Fe)O ferropericlase. At the high pressure-temperature conditions of our planet's deep interior, Fe2+ in ferropericlase undergoes a change in electronic configuration. This pressure-induced transition of iron atoms from high-spin (HS) to low-spin (LS) state is referred to as the iron spin crossover and leads to changes in physical properties of ferropericlase. In particular, a decrease in unit cell volume leads to an anomalous softening of the bulk modulus in the pressure range where HS and LS iron coexists. This directly affects seismic P- and bulk-wave velocities, since they are dependent on the elastic bulk modulus. Therefore, understanding the spin crossover-induced changes in the compressibility of ferropericlase is of vital importance for the interpretation of seismological observations, which are a main source of information about Earth's interior structure. To identify the seismic signal of the spin crossover and detect its occurrence in the lower mantle it is essential to constrain the effects of high temperatures.

Here, we present the first high-temperature measurements of the compressibility of ferropericlase in the spin crossover pressure range [1] using a combination of continuous compression experiments in resistive-heated dynamic diamond-anvil cells and time-resolved X-ray diffraction at beamline P02.2 (PETRA III, DESY). We find that the spin crossover-induced elastic softening of ferropericlase is strongly temperature-dependent. The experimental results are complemented by new theoretical calculations, which are used to produce synthetic seismic tomography models of the lower mantle. This allows us to identify the seismic signature of the spin crossover, providing a tool for its detection in seismic observations. By comparing our synthetic models to data-driven tomographic models, we present new evidence for the presence of the spin crossover in Earth's lower mantle.

[1] Trautner et al. (2023). Compressibility of ferropericlase at high-temperature: Evidence for the iron spin crossover in seismic tomography. *EPSL*, *618*, 118296.

The role of identical charges in enzyme catalysis: Friends or foes?

Kai Tittmann

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The origins of enzyme catalysis have been attributed to both transition-state stabilization as well as ground-state destabilization of the substrate. For the latter paradigm, the enzyme orotidine-5'-monophosphate decarboxylase (OMPDC) serves as a reference system as it contains a negatively charged residue at the active site that is thought to facilitate catalysis by exerting electrostatic stress on the equally charged substrate carboxylate leaving group. Snapshots of how the substrate binds to the active site and interacts with the negative charge had remained elusive. In this talk, I will discuss ultrahigh-resolution crystallographic snapshots of human OMPDC in complex with the genuine substrate, substrate analogues, transition-state analogues and product that defy the proposed ground-state destabilization by revealing that the substrate carboxylate is protonated and forms a favorable low-barrier hydrogen bond with a negatively charged residue. The catalytic prowess of OMPDC mostly results from transition-state stabilization by electrostatic interactions of the enzyme with charges spread over the substrate but also in part from ground-state destabilization through physical distortions of the substrate. Our findings bear relevance for the design of (de)carboxylase catalysts.

DESY Photon Science Users´ Meeting 2024
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Poster Sessions and Industry Exhibition

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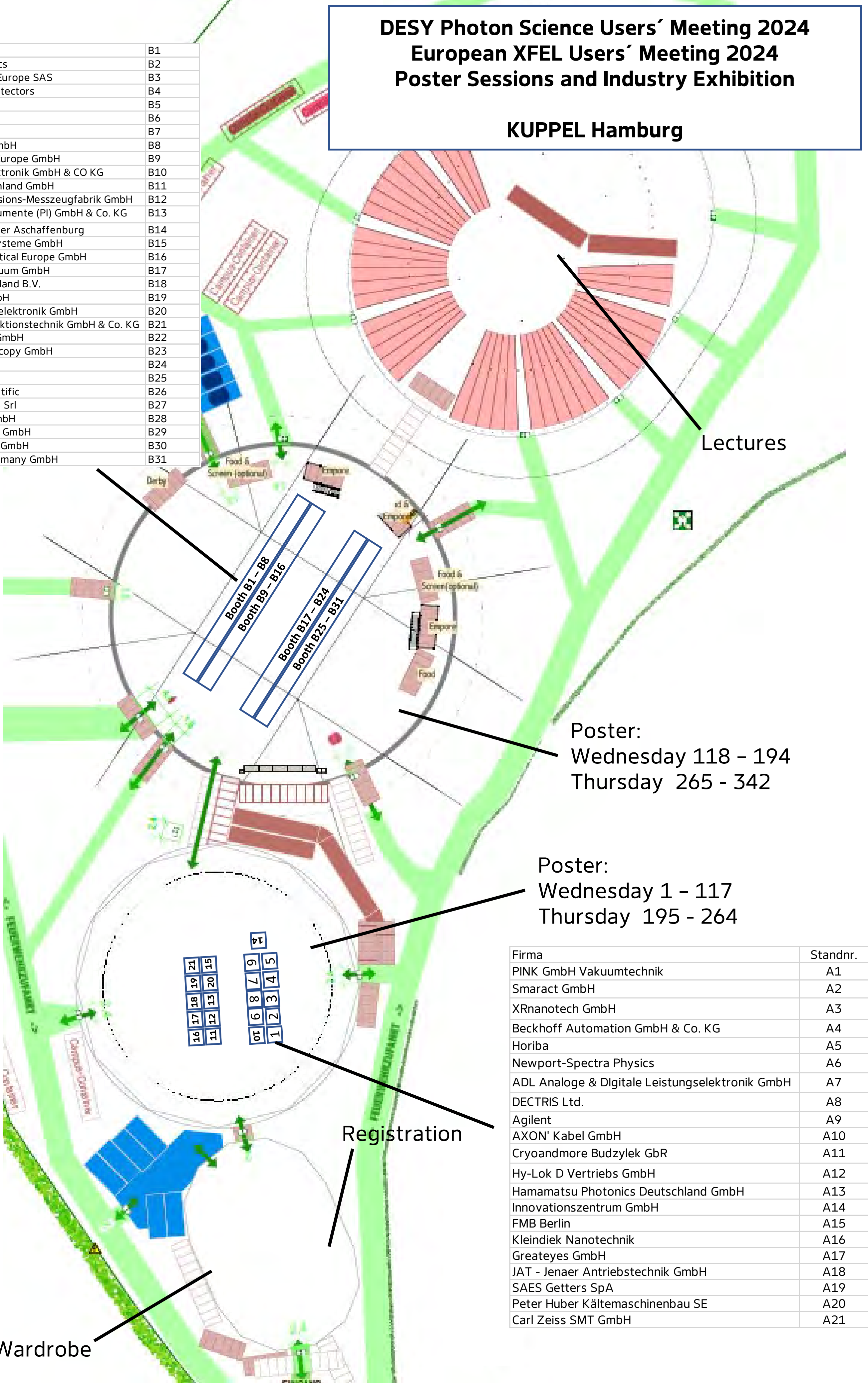

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Information on Future Projects at DESY
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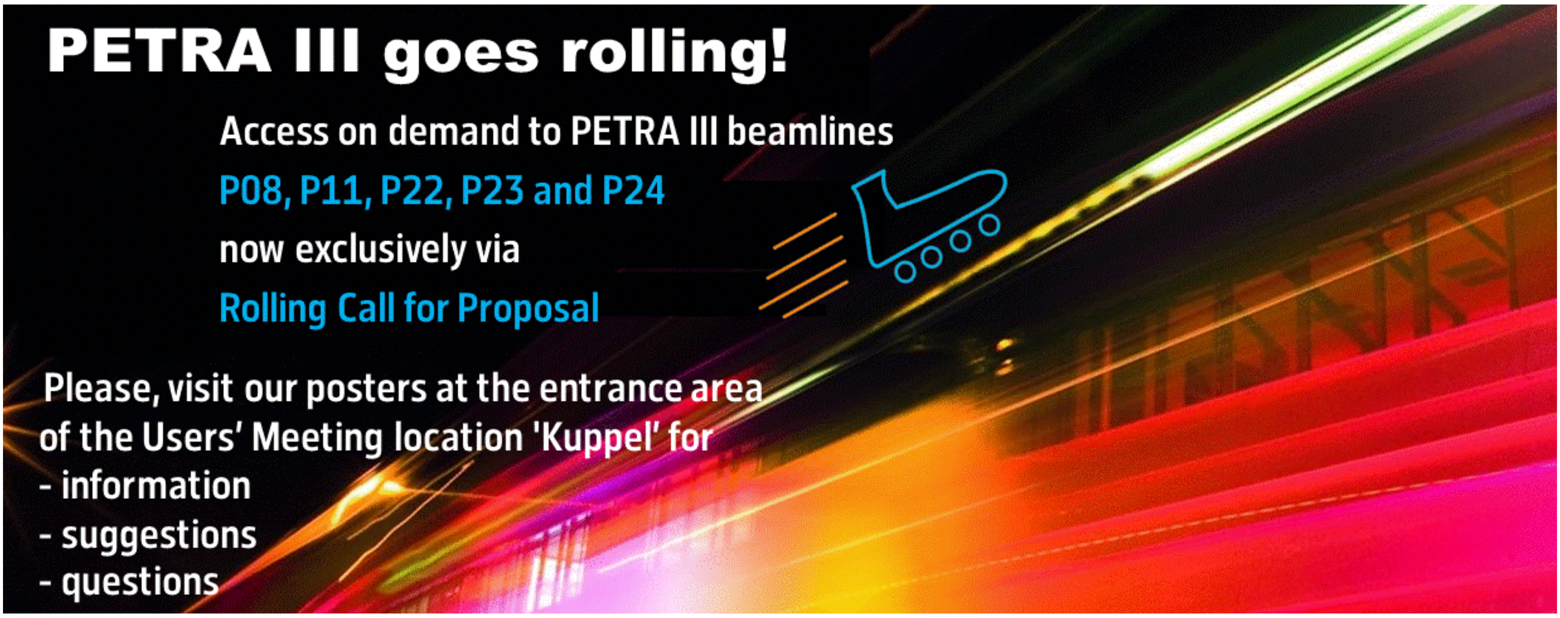

PETRA IV

1) PETRA IV - Update on the Accelerator Complex
2) PETRA IV - Update on the Beamline Portfolio
3) PETRA IV - Civil Construction Projects
4) PETRA IV - Accelerating Sustainability

Information of Campus Partner

DESY-PT
Projektförderung des BMBF zur Erforschung der Materie an Großgeräten
(Project funding by the BMBF for research on matter at large-scale facilities)

II Poster Session Topics

Poster session on Wednesday, 24 January 2024: Posters 1 to 194 (and submitted later)

Poster session on Thursday, 25 January 2024: Posters 195 to 342 (and submitted later)

II.1 European XFEL

1. Upgrade of SASE2 Beamline of European XFEL with Superconducting Afterburner: Potential Photon Output
   C. Lechner, S. Casalbuoni, G. Geloni, E. Schneidmiller, S. Serkez and H. Sinn

2. Observation of fast crystallizations of supercompressed water by using the XFEL combined dynamic diamond anvil cell
   Y.-H. Lee, M. Kim, J. K. Kim, Y. C. Cho and G. W. Lee

3. MS SPIDOC: Mass Spectrometry meets X-ray Single Particle Imaging
   T. Kierspel, A. Kádek, T. Damjanović, J. Kung and C. Uetrecht

4. Ultrafast structural dynamics and lattice response of spin crossover thin films probed with femtosecond electron diffraction and X-ray diffraction.
   D. Vinci, Y. Jiang, R. Schubert, F. Qi, K. Ridier, T. Eklund, P. Zelden, F. Ardana Lamas, C. Deiter, H. Yousef, C. Ott, C. Mariette, M. Lorenc, R. van der Veen, H. Mueller-Werkmeister, R.J. Kaminski, K.N. Jarzembska, D. Xiang and C. Milne

5. Photoelectron spectroscopy laboratory at European XFEL
   I.A. Arkhipushkin and M. Izquierdo

6. Ultrafast dynamics of photoexcited states in Cerium Oxide
   S. Pelatti, E. Spurio, J. S. Pelli Cresi, S. Benedetti, A. di Bona, S. D'Addato, P. Zalden, Y. Jiang, Y. Uemura, H. Wang, D. Vinci, X. Huang, F. Lima, M. Biednov, C. Milne, S. Turchini, P. O'Keeffe, D. Catone, F. Boscherini and P. Luches

7. Sliding charge density waves (CDW) systems under applied current probed by X-ray Free Electron Laser
   D. Ghoneim, A. Gallo-Frantz, E. Bellec, L. Ortega, A. Madsen, V. Jacques and D. Le Bolloc'h

8. Establishing high-quality ultra-fast total scattering & pair distribution function techniques at the European XFEL
   A. F. Sapnik, D. A. Keen and uf-TS/PDF LTP team

9. Tracking light-induced excited state dynamics in molecular systems using ultrafast pump-probe methods
   M. Sekkal, C. Bömer, M. Busi, T. Choi, S. J. Goodner, Z. Nurekeyev, F. Otte, R. D. Schaller, K. Haldrup, D. J. Gosztola, M. Kushniyarov, C. Bressler and K. Kubicek

10. Origins of enhanced aurophilicity in stimuli-responsive dimer complexes using Hard X-Ray WAXS and HERFD-XAS
    S. Paul Dutta, D. Khakhulin, D. Koziej and C. Milne

11. Resonant X-ray excitation of the nuclear clock isomer Scandium-45
    Y. Shvyd'ko, R. Röhlsberger, O. Kocharovskaya, J. Evers, G. Geloni, P. Liu, D. Shu, A. Miceli, B. Stone, W. Hippler, B. Marx-Glowna, I. Uschmann, R. Loetzsch, O. Leupold, H.-C. Wille, I. Sergeev, M. Gerharz, X. Zhang, Ch. Grech, M. Guetg, V. Kocharyan, N. Kujala, S. Liu, W. Qin, A. Zozulya, J. Hallmann, U. Boesenberg, W. Jo, J. Möller, A. Rodriguez-Fernandez, M. Youssef, A. Madsen and T. Kolodziej

12. Utilising the EuXFEL to characterise material response to laser imprint
    B. Fisher and N. Woolsey

13. Picosecond surface morphology in femtosecond laser irradiated metals investigated by GID and GISAXS
Ö. Öztürk, D. Ksenzov, L. Randolph, S.V. Rahul, M. Banjafar, L. Huang, J.P. Schwinkendorf, T. Kluge, M. Nakatsutsumi and C. Gutt

14. The Femtosecond X-ray Experiments (FXE) Instrument at the European XFEL
D. Bregenholt Jakobsen, F. Alves Lima, F. Ardana-Lamas, M. Biednov, P. Frankenberger, S. Haryati, X. Huang, Y. Jiang, D. Khakhulin, M. Knoll, S. Paul Dutta, D. Vinci, Y. Uemura, H. Wang, H. Yousef, P. Zalden and C. Milne

15. Microsecond time-resolved X-ray scattering by utilizing MHz repetition rate at second-generation XFELs
P. E. Konold, L. Monrroy, A. Bellisario, D. Filipe, P. Adams, R. Alvarez, R. Bean, J. Bielecki, S. Bódizs, G. Ducrocq, H. Grubmueller, R. A. Kirian, M. Kloos, J.C.P. Koliyadu, F.H.M. Koua, T. Larkiala, R. Letrun, F. Lindsten, M. Maihöfer, A. V. Martin, P. Mészéros, J. Mutisya, A. Nimmrich, K. Okamoto, A. Round, T. Sato, J. Valerio, D. Westphal, A. Wollter, T.V. Yenupuri, T. You, F. Maia and S. Westenhoff

16. Photo Electron Spectrometers for Non-Invasive Photon Diagnostics at the European XFEL
J. Laksman, F. Dietrich, T. Maltezopoulos, J. Liu, D. de Lima, N. Kujala and J. Grünert

17. Mechanical design and integration of the SXP scientific instrument at the European XFEL
V. Vardanyan, P. Grychtol, E. Tikhodeeva, D. Doblas-Jimenez, J. Ohnesorge, N. Kohlstrunk, J. Buck, S. Thiess, M. Dommach, D. La Civita, M. Vannoni, K. Rossnagel, G. Schönhense, S. Molodtsov and M. Izquierdo

18. Resonant inelastic x-ray scattering beyond the SASE resolution limit
A. Forte, T. Gawne, K. K. Alaa El-Din, O. S. Humphries, T. R. Preston, C. Crépisson, T. Campbell, P. Svensson, S. Azadi, P. Heighway, Y. Shi, D. A. Chin, E. Smith, C. Baehtz, V. Bouffetier, H. Höppner, D. McGonegle, M. Harmand, G. W. Collins, J. S. Wark, D. N. Polsin and S. M. Vinko

19. Probing Pre-Hydrate Cage Formation
R.P.C. Bauer, A. Gierke, C. Goy, J. Valerio, L. Adriano, J.-E. Pudell, W. Jo, J. Möller, N.N. Striker, N.C. Giesselmann, S.C. Hoevelmann, W. Roseker, K. Ayyer, C. Sternemann, R. Grisenti, J. Schultz and F. Lehmkühler

20. New developments of liquid sample delivery at EuXFEL
J. Valerio, E. Delmas, K. Dörner, H. Han, M. Kloos, A. Wrona and J. Schulz

21. Optimizing VLS Grating Design for SASE Spectrometer
Y. Zhong, J. Feng, M. Wu, J. Cai and W. Zhang

22. High-field laser-based THz sources at European XFEL
I. Radu, R. Ivanov, B. Monoszlai, D. Rompotis, J. Meier, R. Secareanu, M. Emons, R. Fabbri, D. Kane, S. Venkatesan, J. Wang, U. Wegner and M. Lederer

23. Exploring elastic scattering enhancement via transient resonances probed by x-ray superfluorescence
D. Ronchetti, A. Benediktovitch, A. Leonau, S. Chuchurka, V. Sukharnikov, E. Zavatti, A. Halavanau, N. Welke, U. Bergmann, J. Bielecki, J. Koliyadu and N. Rohringer

24. Femtosecond time-resolved L-edge XAS in solution at EuXFEL: Application to the photophysics of Cyanocobalamin
N. Ghodrati, L. Adriano, C. Carinan, R. Carley, Y.-P. Chang, C. Danilevski, C. David, R. Engel, N. Gerasimova, L. Le Guyader, M. Harder, N. Huse, R. M. Lamb, T. Mamyrbayev, T. P. McClain, L. Mercadier, A. Mukherjee, J. E. Penner-Hahn, M. Porro, A. Scherz, R. J. Sension, M. Teichmann, M. Turcato, J. Valerio, R.-P. Wang, Z. Yin and B. E. Van Kuiken

25. X-ray spectroscopy simulations of highly correlated materials at European XFEL
N. Brouwer and A. Lichtenstein

26. EXtra-Xwiz: A Tool to Streamline Serial Femtosecond Crystallography Workflows at European XFEL
O. Turkot, F. Dall'Antonia, R. J. Bean, J. E, H. Fangohr, D. E. Ferreira de Lima, S. Kantamneni, H. J. Kirkwood, F. H. M. Koua, A. P. Mancuso, D. V. M. Melo, A. Round, M. Schuh, E. Sobolev, R. de Wijn, J. J. Wrigley and L. Gelisio

27. Non-linear multiphoton excitation and ionization of highly charged ions using high intensity XFEL pulses
M. Togawa, M. Botz, J. Danisch, J. Goes, Z. Harman, K. Koebnick, K. Kubicek, M. Leutenegger, C. Lyu, M. Maxton, A. Mohamed, T. Pfeifer, M. Sekkal, C. Shah, J. R. Crespo López-Urrutia, M. Meyer and T. M. Baumann

28. Single-Shot Wavefront Characterisation at the European XFEL
T. W. Guest, R. Bean, G. van Riessen, A. Mancuso and B. Abbey

29. X-ray optical pulse arrival monitor based on spintronic THz emitters
R. Carley, L. Mercadier, J. Liu, L. Le Guyader, M. Teichmann, M. Gensch, T. Kampfrath, T. Seifert, I. Radu, R. Ivanov, S. Parchenko, L. P. Hoang, G. Mercurio, G. Merzoni, T. Citra Asmara, Y.-P. Chang and A. Scherz

30. Femtosecond Single-Particle Diffractive Imaging of Giant-Hemeprotein with XFEL Pulses
P. L. Xavier, A. Morgan, S. Dold, J. Bielecki, A.Samanta, A. Estillore, C. Li, W. Zhang, M. Butola, E. Chia, N. Ivanov, E. Soblev, L. Gelisio, P. Schmidt, F. Dall'Antonia, I.D.G. Aquino, S. Rafie-Zinedine, F. Koua, R. Bean, C. Danilevski, M. Porro, L. Worbs, M. Vakilli, A. Keloth, L.V. Haas, J. He, K. Janson, O. Yefanov, C. Schmidt, E. Round, M. Kloos, J. Schulz, Y. Ovcharenko, R. Boll, T. Mazza, S. Usenko, B. Senfftleben, A.D. Fanis, F. Maia, J. Kuepper, S. Bajt, A.V. Martin, N.D. Loh, M. Meyer and H.N. Chapman

31. Femtosecond Single-Particle Diffractive Imaging of Computationally Designed De Novo Protein Complexes with XFEL Pulses
P. L. Xavier, E.C. Yang, A. Morgan, S. Dold, J. Bielecki, A. Samanta, A. Estillore, C. Li, W. Zhang, M. Butola, E. Chia, N. Ivanov, E. Soblev, L. Gelisio, P. Schmidt, F. Dall'Antonia, I.D.G. Aquino, M. Miranda, S. Rafie-Zinedine, F. Koua, R. Bean, C. Danilevski, M. Porro, L. Worbs, M. Vakilli, A. Keloth, L.V. Haas, J. He, K. Janson, O. Yefanov, C. Schmidt, E. Round, M. Kloos, J. Schulz, Y. Ovcharenko, R. Boll, T. Mazza, S. Usenko, B. Senfftleben, A.D. Fanis, F. Maia, J. Kuepper, S. Bajt, A.V. Martin, N.D. Loh, M. Meyer, S. Ovchinnikov, N.King, D. Baker and H.N. Chapman

32. Direct observation of electron relaxation dynamics in a warm dense plasma.
Y. Shi

33. Interpretable Machine Learning at the EuXFEL
D. Ferreira de Lima, A. Majid and L. Gelisio

34. Mix-and-Extrude using 3D printed nozzle: towards time-resolved membrane protein crystallography
H. Han, M. Vakili, C. Schmidt, A. Wrona, M. Kloos, I. de Diego, K. Dörner, T. Geng, C. Kim, F. Koua, D. Melo, M. Rappas, A. Round, E. Round, M. Sikorski, J. Valerio, T. Zhou, K. Lorenzen and J. Schulz

35. Resonant double core hole spectroscopy of ultrafast decay dynamics in Fe complexes
J. Schwarz, M. Nissen, A. De Fanis, A. Rörig, K. Baev, F. Trinter, T. Laarmann, N. Huse, P. Wernet, M. Meyer, T. Baumann, S. Dold, T. Mazza, Y. Ovcharenko, S. Usenko, M. Ilchen, A. Prystawik, H. Wikmark and M. Martins

36. Imaging Distribution of Molecular Structures with Coulomb Explosion Imaging
B. Richard, R. Boll, R. Santra, L. Inhester and T. Jahnke

37. Structure-dynamics correlation during ultrafast melting of a polycrystylline palladium metal
A. Olczak, P. Dziegielewski, S. Khan, Z. Kostera, K.P. Migdal, I. Milov, R. Sobierajski, V.V. Zhakohovski and J. Antonowicz

38. APPLE-X: Magnetic measurements after the repair
U. Englisch, S. Karabekyan, M.Yakopov, S.Casalbuoni, S. Abeghyan, M. Calvi, Th. Schmidt, F. Preiskorn and M. Bagha-Shanjani

39. The new scientific data policy for European XFEL
F. Dall'Antonia, J. Malka, L. Gelisio, P. Schmidt, E. Sobolev, G. Winterhoff and K. Wrona

40. The concept of Data Management Plans for European XFEL proposals
F. Dall'Antonia, J. Malka, L. Gelisio, D. Goeries, S. Hauf, L. Maia, P. Schmidt and K. Wrona

41. Mössbauer science with ^{57}Fe at X-ray free-electron lasers
M. Gerharz and J.Evers for the ^{57}Fe EuXFEL collaboration

42. Liquid Sample Delivery for Time-Resolved Coherent Diffractive Imaging at X-ray Free-Electron Lasers
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43. Dehydration of MS2 bacteriophage observed through X-ray single particle imaging via unsupervised deep learning
A. Mall, A. Munke, Z. Shen and K. Ayyer

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X. Huang, Y. Uemura, F. Ardana-Lamas, P. Frankenberger, M. Knoll, H. Yousef, H. Wang, M. Nachtegaal, L. Wang, C. Milne and F. A. Lima

45. 'Show Me How' - Meeting and Exceeding Reproducibility Requirements
R. Rosca

46. MHz beam sweeping serial crystallography for high-throughput pharmaceutical screening
A. C. Rodrigues, M. Galchenkova, M. Barthelmess, P. Reinke, P. Fischer, S. Guenther, S. Falke, A. Tolstikova, V. Hennicke, J. Meyer, S. T. Veedu, O. Yefanov, T. Pakendorf, L. Gumprecht, H. Chapman and A. Meents

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B. Senfftleben, R. Boll, T. Baumann, V. Bondar, H. Bromberger, A. De Fanis, S. Dold, B. Erk, T. Mazza, J. Montaño, T. Mullins, Y. Ovcharenko, A. Parenti, N. Rennhack, D. Rivas, P. Schmidt, M. Shokr, S. Trippel, S. Usenko and M. Meyer

48. Status of FAST-XPD: Photon data base for the European XFEL and FLASH
M. Manetti, L. Samoylova, H. Sinn, J. Szuba, K. Wrona, M. Yurkov and I. Zagorodnov

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J. Choi, R. Husband, H. Hwang, T. Kim, Y. Bang, S. Yun, J. Lee, H. Sim, Y. Jung, L. Andriambariarijaona, O. Ball, J. McHardy, M. McMahon, S. Ninet, C. Sanchez-Valle, X. Li, A. Mondal, K. Appel, R. Briggs, J. Buchen, V. Cerantola, S. Chariton, A. Coleman, H. Cynn, F. Datchi, E. Edmund, J. Eggert, L. Ehm, W. Evans, G. Fiquet, M. French, M. Frost, K. Glazyrin, A. Goncharov, S. Hau-Riege, L. Huston, T. Hutchinson, Z.Z. Jenei, J. Kim, M. Kim, E. Koemets, Z. Konopkova, M. Lipp, P. Loubeyre, H. Marquardt, E. McBride, G. Morard, E. O'Bannon, R. Occelli, E. Pace, J. Pigott, V. Prakapenka, C. Prescher, C. Pépin, R. Redmer, R. Smith, C. Storm, C. Strohm, B. Sturtevant, N. Velisavljevic, C.-S. Yoo, U. Zastrau, S. Kim, D. Nam, R. S. McWilliams, H.-P. Liermann and Y. Lee

50. Sample delivery methods at European XFEL – User support by the SEC group
K. Dörner, I. Arkhipushkin, V. Bazhenov, I. de Diego, E. Delmas, C. Deiter, H. Han, M. Kittel, M. Kloos, J. Moore, S. Rafie-Zinedine, E. Round, C. Schmidt, R. Schubert, P. Smyth, M. Vakili, J. Valerio, A. Wrona, J. Bielecki and J. Schulz

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C. Deiter, I. Arkhipushkin, V. Bazhenov, I. de Diego, E. Delmas, K. Dörner, H. Han, M. Kittel, M. Kloos, J. Moore, S. Rafie-Zinedine, E. Round, C. Schmidt, R. Schubert, P. Smyth, J. Valerio, A. Wrona, J. Bielecki and J. Schulz

52. Demonstration of MHz X-ray Photon Correlation Spectroscopy using acoustic levitator at European XFEL
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53. DAMNIT: Automated experiment overview
C. Carinan, M. do Carmo Teodoro, T. Kluyver, T. Michelat, R. Rosca, J. Wrigley and L. Gelisio

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R. Bean, L. Bubacco, P. Mariani, V. Minicozzi, S. Morante, M.G. Ortore, M. Polentarutti, N. Plotegher, M. Sandre, F. Spinozzi and F. Stellato

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R. Loetzsch, F. Sommer, W.Hippler, K.S. Schulze, B. Marx-Glowna, I.Uschmann and G.G. Paulus

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A. Chretien, M. F. Nagel, S. Botha, R. de Wijn, L. Brings, K. Dörner, H. Han, J. C. P. Koliyadu, R. Letrun, A. Round, T. Sato, C. Schmidt, R. Secareanu, D. von Stetten, M. Vakili, A. Wrona, R. Bean, A. Mancuso, J. Schulz, A. R. Pearson, T. Kottke, K. Lorenzen and R. Schubert

58. Thermal conductivity of water ice at planetary interiors conditions
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59. Data Management Infrastructure for European XFEL.
J. Malka, S. Aplin, D. Boukhelef, K. Filippakopoulos, L. Maia, T. Piszczek, G.Previtali, J. Szuba, K. Wrona, S. Dietrich, M. Gasthuber, J. Hannappel, M. Karimi, Y. Kemp, R. Lueken, T. Mkrtchyan, K. Ohrenberg, K.Schwarz, F. Schluenzen, P. Suchowski and Ch. Voss

60. Plasma instabilities can be probed with X-ray scattering!
P. Ordyna, C. Bähtz, E. Brambrink, M. Bussmann, A. Garcia, M. Garten, L. Gaus, J. Grenzer, C. Gutt, H. Höppner, L. Huang, O. Humphries, B. Marré, J. Metzkes-Ng, M. Nakatsutsumi, Ö. Öztürk, X Pan, F. Paschke-Brühl, A. Pelka, I. Prencipe, T. Preston, L. Randolph, H. Schlenvoigt, J. Schwinkendorf, M. Šmíd, S. Starke, R. Stefanikova, E. Thiessenhusen, T. Toncian, K. Zeil, U. Schramm, T. Cowan and T. Kluge

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D. Hammer, K. Ahmed, I. Bermudez, C. Carinan, C. Danilevski, T. Kluyver, T. Michelat, R. Rosca, E. Sobolev, J. Wrigley, L. Gelisio and P. Schmidt

62. The EuXFEL Outreach Program for Young Scientists - Expanding the EuXFEL User Base
E. Round, J. Pivonkova, A. Bonucci and J. Schulz

63. Ultrafast light-induced dynamics of polarization and strain in a ferroelectric thin film
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H. Han, I. Arkhipushkin, V. Bazhenov, A. Chretien, I. de Diego, E. Delmas, C. Deiter, K. Dörner, M. Kittel, M. Kloos, K. Lorenzen, J. Moore, S. Rafie-Zinedine, E. Round, C. Schmidt, R. Schubert, P. Smyth, J. Valerio, A. Wrona and J. Schulz

65. Diagnosing relativistic plasma surfaces using GISAXS
M. Banjafar and S V Rahul

66. Magnetic and cryogenic sample environment at the MID instrument
J.D. Moore, S. Schulz, A. Madsen, P. Zalden and F. Alves Lima

67. Thermal and non-thermal decomposition of lead iodide: material damage induced by XUV/x-ray lasers and other radiation sources
A. Horynova, V. Hajkova, S. Jelinek, J. Chalupsky, V. Vozda, L. Vysin, J. Bulicka, T. Burian, R. Dudzak, M. Krupka, J. Krasa, N. Medvedev and L. Juha

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L. Maia, K. Wrona, M. Manetti, I. Derevianko, V. Singh, B. Vanganuru, J. Szuba, J. Malka and G. Previtali

69. Heisenberg RIXS instrument at SCS, European XFEL for ultrafast spectroscopy studies on quantum materials
S. Parchenko, L. Adriano, A. Alic, D.R. Baykusheva, R. Carley, G.S. Chiuzbaian, M.P. Dean, O. Duros, A. Foelisch, M. Foerst, B.K. Freelon, N. Gerasimova, G. Ghiringhelli, X. Jiang, D. Jost, M. Kusch, T. Laarman, V. Lebedev, W.-S. Lee, C.Y. Liu, L. Martinelli, G. Merzoni, L. Mercadier, M. Minola, M. Mitrano, S. Molodtsov, C.S. Pathiraja, J.N. Ranhili Pelige, Y.Y. Peng, Q. Qiu, T. Schmitt, J. Sears, S. Sreenkatan Nair Lalithambika, S. Techert, M. Teichmann, S. Ten Huisen, B. van Kuiken, Z. Yin, A. Scherz and J. Schlappa

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S. Palutke, R.-M. Wheater, H. Yousef, M. Bishop, M. Ramilli, M. Hart, D. Khakhulin, X. Huang, C. Milne, M. Turcato and M. Veale

71. SimEx-Lite: easy access to start-to-end simulation for experiments at advanced light sources
J. E, C. Fortmann-Grote, E. Sobolev, L. Gelisio and R. Bean

72. Characterization of a Single Module of DEPFET X-Ray Camera at the European XFEL
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C. Neuhaus, J. Alfken, M. Stammer, SPB Team EuXFEL, M. Ganzella, R. Jahn and T. Salditt

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75. The Influence of Parallax Effects in Thick Silicon Sensors on Coherent Diffraction Imaging
M. Kuster, R. Hartmann, S. Hauf, P. Holl, T. Rüter and L. Strüder

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K. Cheung, A. Rouzée, C. P. Schulz, T. Jahnke, J. McManus, T. Walmsley, S. Kellerer, I. Makos, D. Busto, P. Eng-Jonsson, F. Allum, M. Burt, C. Vallance, R. Boll, F. Rodriguez Diaz, J. Mikosch, T. Witting, Z.-Y. Zhang, A. Rudenko, H. Stapelfeldt, M. J. J. Vrakking, O. Grob, S. M. Leinberger, K. Borne, K. Ueda, C.-S. Lam, S. Usenko, B. Senfftleben, T. Mazza, T. Baumann, T. Martinez, G. Sansone, D. Rolles, M. Meyer, M. Brouard, T. Mullins and K. Amini

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T. C. Yıldız, J. Lu, W. Freund, D. Khatkhulin, H. Yousef, C. Milne and J. Grünert

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K. Tasca, U. Bösenberg, J. Hallman, A. Madsen, J. Moore, J. Pudell, A. Rodriguez-Fernandez, R. Shayduk, M. Vannoni, J. Wonhyuk, A. Zozulya and L. Samoylova

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S. Marotzke, A. Philippi-Kobs, D. Lott, M. Riepp, L. Le Guyader, L. Müller, W. Roseker, R. Frömter, K. Chen, G. Mercurio, L. P. Hoang, S. Parchenko, R. Carley, A. Scherz, F. Radu, G. Grübel, M. Beye and K. Rossnagel

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M. Dargasz, N. D. Anthuparambil, A. Girelli, M. Bin, M. Kowalski, S. Retzbach, S. Timmermann, J. Savelkouls, M. Raza, I. Andronis, M. Filianina, A. Ragulskaya, N. Begam, Y. Chushkin, T. Seydel, M. Paulus, U. Boesenberg, J. Hallmann, J. Möller, A. Rodriguez-Fernandez, R. Shayduk, W. Jo, J.E. Pudell, A. Zozulya, A. Madsen, F. Schreiber, F. Zhang, F. Perakis and C. Gutt

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S. Fridman, H. Graafsma, H. Hirsemann, A. Klyuev, S. Lange, T. Laurus, D. Magalhaes, A. Marras, S. Schneider, O. Shefer-Shalev, S. Stern, T. Stoye and U. Trunk

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85. Three steps towards a broader bilateral scientific cooperation between the European XFEL facility and its Italian current and perspective users.
F. Boscherini and M. Izquierdo, P. Luches, T. Mazza, M. Meyer, C. Milne, R. Mincigrucci, G. Panaccione and P. Piseri

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A. Rörig, T. Mazza, S. Fritzsche, T. M. Baumann, A. De Fanis, S. Dold, B. Senfftleben and M. Meyer

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L. Funke, S. Savio, A. Held, L. Wülfing, N. Wieland, K. Dingel, T. Otto, R. Hindriksson, L. Marder, C. Passow, P. Rupprecht, A. Schletter, P. Walter, J. Grünert, J. Liu, T. Baumann, R. Boll, A. De Fanis, S. Dold, T. Mazza, J. Montaño, D. Raiser, D. Rivas, P. Schmidt, M. Meyer, T. Mullins, M. Ilchen and W. Helml

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B. E. Van Kuiken, L. Adriano, R. Carley, Y. P. Chang, C. Carinan, C. Danilevski, C. David, D. Diaman, S. Eckert, A. Foehlisch, N. Gerasimova, N. Ghodrati, R. Lamb, L. Le Guyader, Y. Harada, J. Harich, N. Huse, R. Jay, T. Laarmann, T. Mamyrbayev, E. McClain, L. Mercadier, A. Mukherjee, J. Niskanen, J. Penner-Hahn, A. Pietzsch, M. Porro, T. Reuss, A. Scherz, J. Schlappa, R. Sension, S. Sreekantan, S. Techert, M. Teichmann, M. Turcato, K. Ueda, R. Uglino, J. Valerio, V. Vaz da Cruz, R.-P. Wang, P. Wernet, H. Wikmark, H. J. Woerner, W. Xu and Z. Yin

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M. Tavakkoly, J. Chalupsky, J. Grünert, V. Hajkova, W. Hillert, S. Jelinek, L. Juha, A. Koch, D. La Civita, M. Makita, M. Meyer, M. Planas, S. Serkez, H. Sinn, V. Vozda, T. Wohlenberg and M. Vannoni

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95. Single-shot temporal characterization of XUV FEL@FLASH
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H. Lindenblatt, K. Schnorr, S. Augustin, S. Meister, F. Trost, P. Schoch, G. Schmid, Y. Liu, M. Braune, M. Kuhlmann, R. Treusch, C. D. Schröter, T. Pfeifer and R. Moshammer

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98. New wavefront sensor for renewed differential pumping unit at FLASH2 beamlines
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99. Miniature ultra-broadband spectrometer for Mid-IR and THz range
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100. New insights into the laser-assisted photoelectric effect from solid state surfaces.
L. Wenthaus, F. Roth, N. Kabachnik, M. Borgwardt, S. Düsterer, D. Kutnyakhov, D. Pototochin, S. Palutke, N. Wind, F. Pressacco, M. Scholzu, G. Brenner, O. Gessner, S. Molodtsov and W. Eberhardt

101. Endstation for time-resolved x-ray photoemission spectroscopy at FELs.
L. Wenthaus, D. Kutnyakhov, H. Meyer, S. Gieschen and M. Martins

102. Ultrafast dynamics of Azobenzene: a soft x-ray approach
F. Lever, D. Mayer, H. Cankaya, G. Cirmi, T. Driver, S. Duesterer, U. Fruehling, G. Goetzke, R. Ingle, E. Isele, M. Martins, A. Tul Noor, S. Palutke, J. Schwarz, J. Wang and M. Gühr

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A. Azzolin, O. Cannelli, J. Hahne, M. Seitz, A. bin Wahid, K.F. Wong, V. J. Yallapraganda, E. Appi, M. Braunem, S. Duesterer, N. Dudovich, U. Fruehling, C. Heyl, M. Kovacev, T. Lang, U. Morgner, R. Moshammer, D. Oron, C. Ott, C. Papadopoulou, T. Pfeifer, E. Schneidmiller, E. Maasson, V. Wanie, A. Trabattoni and F. Calegari

104. The status of the intense THz source and beamline at FLASH
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105. In-situ femtosecond time-resolved X-ray photoelectron spectroscopy studies of charge carrier dynamics underlying photocatalytic water splitting
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S. Dziarzhytski, M. Sinha, L. Wenthaus, D. Kutnyakov, R. Engel, J. Schunck, R.-P. Wang S, Marotzke, N. Wind, M. Scholz, N. Huse, F. Pressacco, M. Beye, E. Ploenjes-Palm and G. Brenner

107. FEL and HHG-based time-of-flight momentum microscopy: 3 time-resolved photoemission modalities in 1 experiment
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108. Sub-50 fs temporal resolution in an FEL-optical laser pump-probe experiment at FLASH2
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109. PESdata: graphical user interface for analysis of multidimensional photoemission spectroscopy data measured at FELs and synchrotrons and laboratory setups
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110. A set-up for liquid-phase soft X-ray absorption and emission spectroscopy
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111. Probing the Dynamics in Liquids by XUV-THz Pump-Probe Electron Spectroscopy (DYLIXUT)
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112. Time resolved spectroscopy at the interface of water/oxide
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113. Electronic molecular movies at FLASH
M. Gühr, S. Alisauskas, A. Azzolin, F. Calegari, H. Cankaya, G. Cirmi, S. Düsterer, R. Feifel, U. Frühling, G. Goetzke, I. Hartl, R. Ingle, M. Kuhlmann, F. Lever, M. Martins, D. Mayer, S. Paluttke, D. Picconi, P. Saalfrank, S. Schulz, J. Schwarz, R. Squibb, A. Trabattoni and A. Tul-Noor

114. Machine learning analysis of single-shot X-ray pulse data from a transverse deflecting cavity
G. Goetzke, F. Möller, T. Otto, C. Gerth, E. Schneidmiller, J. Roensch-Schulenburg, M. Vogt, C. Behrens, S. Düsterer and G. Hartmann

115. An upgraded XUV and soft X-ray split-and-delay unit for FLASH1
M. Dreimann, F. Wahlert and H. Zacharias

II.3 Other topics, external facilities and theory

116. snip - user centric collaborative digital lab book
M. Osterhoff, S. Mohr, J. P. Burchert, T. Salditt and S. Köster

117. Transient core-hole screening observed by time-resolved X-ray absorption spectroscopy at the Zn K-edge of ZnO: experiment and theory
T.C. Rossi, L. Qiao, C.P. Dykstra, R. Wallick, J.H. Burke, E. Nicholas, A.M. March, G. Doumy, B. Buchholz, K. Gilmore, R. Rodrigues Pelà, C. Draxl and R.M. van der Veen

118. Synchrotron radiation study of phase transition in vanadium dioxide based thin films
M. Kumar, S. Rani and H. H. Lee

119. Detecting nonlinear and many-body dynamics in nuclear quantum optics
L. Wolff and J. Evers

120. Theoretical description of x-ray absorption spectroscopy of excitons
N. Farahani and D. Gorelova

121. Sn/SnO2 x Nanostructures Engineering
P. Liu, M. A. van Spronsen, A. Makarova, S. Turishchev and V. Sivakov

122. NFFA European piolet (NEP)
J. Dwivedi, T. F. Keller and A. Stierle

123. The DESY NanoLab
H. Noei, T. F. Keller, V. Vonk, R. Röhlsberger and A. Stierle

124. Data processing for X-ray detectors
D. Pennicard, V. Rahmani and H. Graafsma

125. Ultrafast dynamical diffraction in single crystal to study lattice distortions
A. Rodriguez-Fernandez

126. Investigating Nanometric Ultrafast Surface Dynamics Beyond the Laser-Irradiation Zone with Grazing Incidence Small Angle X-ray Scattering (GISAXS)
M. Banjafar, S.V. Rahul, L. Randolph, T. R. Preston, J.P. Schwinkendorf, M. Makita, T. Yabuuchi, N. Mamiko, K. Miyanishi, L. Huang, T. E. Cowan, C. Gutt, T. Kluge and M. Nakatsutsumi

127. Classical Molecular Dynamics Simulations of Surface Modifications Triggered by a Femtosecond Laser Pulse
V. Lipp and B. Ziaja

128. Size dependent viscosities in water probed by XPCS
N. N. Striker, F. Schulz, C. Goy, F. Caupin and F. Lehmkühler

129. Helmholtz Imaging
P. Heuser

130. Laser-induced alignment of nanoparticles and macromolecules
L. Haas, X. Cheng, M. Amin, A. Samanta and J. Kuepper

131. Femtosecond X-ray and Optical Pump-Probe studies of aqueous Cl and Br and I
Z. Nurekeyev, M. Sekkal, H. Hwang, K. Kubicek and C. Bressler

132. Time-resolved Hard X-ray Emission Spectroscopies using Self-seeded Pulses at PAL-XFEL
T.-K. Choi, J. Park, G. Kim, H. Jang, S.-Y. Park, J. H. Sohn, B. I. Cho, H. Kim, K. S. Kim, G. Park, H. Choi, D. Jang, M. Kim, I. Eom, I. Nam and S. H. Chun

133. Computational study of diffraction image formation from XFEL irradiated single ribosome molecule
M. Stransky, J. E, Z. Jurek, R. Santra, R. Bean, B. Ziaja and A. P. Mancuso

134. Helmholtz Imaging DESY
S. Kabri, L. Kuger, L. Weigand, T. Roith and M. Burger

135. THz FEL at PITZ: Status and Perspectives
M. Krasilnikov, N. Aftab, Z, Amirkhanyan, D. Dmitriiev, J. Good, A. Grebinyk, M. Gross, A. Hoffmann, D. Kalantaryan, M. Kelisani, E. Kongmon, X.-K. Li, Z. Lotfi, A. Lueangaramwong, S. Mohanty, A. Oppelt, C. Richard, F. Riemer, E. Schneidmiller, F. Stephan, G. Vashchenko, D. Villani, M. Yurkov, S. Zeeshan and X. Zhang

136. Measurement of the density evolution of laser-heated gold using single shot X-ray diffraction at an XFEL
A. Descamps, M. Schörner, B. K. Ofori-Okai, O. Bistoni, Z. Chen, E. Cunningham, L, B. Fletcher, N. J. Hartley, J. B. Hastings, D. Khaghani, M. Mo, B. Nagler, V. Recoules, R. Redmer, D. G. Senesky, P. Sun, H-E Tsai, T. G. White, S. H. Glenzer and E. E. McBride

137. Shock-frozen beams of biomolecules and nanoparticles for single particle imaging
J. He, A. D. Estillore, K. Janson, S. K. Peravali, A. K. Samanta, P. Neumann, M. Breuer and J. Küpper

138. Ultrafast X-ray induced magnetization dynamics in Co and Ni
K.J. Kapcia, V. Tkachenko, F. Capotondi, A. Lichtenstein, S. Molodtsov, L. Mueller, A. Philippi-Kobs, P. Piekarz and B. Ziaja

139. Percival: 2 Megapixels for soft X-rays – recent user experiments and next steps
M. Hajheidari, J. Correa, A. Marras, C.B. Wunderer, T. Hirono, J.Gebert F. Krivan, S. Lange, I. Shevyakov, V. Vardanyan, N. Guerrini, B. Marsh, I. Sedgwick, G. Cautero, D. Giuressi, R.H. Menk, A. Greer, T. Nicholls, W. Nichols, U. Pedersen, M. Nakhostin, N. Tartoni, H.J. Hyun, S.H. Kim, S.Y. Park, K.S. Kim, F. Orsini, F.J. Iguaz, and H. Graafsmaa, M. Mehrjoo, R. Battistelli, F. Lehmkühler, M. Hoesch, K. Bagschik, F. Büttner, B. Pfau, E. Plönjes, K. Kharitonov, M. Ruiz-Lopez, R. Pan, S. Gang and B. Keitel

140. Imaging Ultrafast Chemical Dynamics
S. Trippel and J. Küpper

141. A mutiscale simulation methodology for nano particle injection through aerosol injectors
S.K. Peravali, A.K. Samanta, M. Amin, J. Küpper, P. Neumann and M. Breuer

142. Sub-cycle Synthesized IR Waveforms for HHG and Attosecond Science
G. M. Rossi, F. Scheiba, M. A. Silva-Toledo, M. Kubullek, R. E. Mainz and F. X. Kärtner

143. Direct Conversion Of Ionizing Radiation Into Electrical Energy Using PIN Diodes
S. Ilić, M. Sarajlić, S. Stanković and D. Vasiljević-Radović

144. Complete imaging of the reaction pathways of ionized water dimer
I. S. Vinklárek, H. Bromberger, N. Vadassery, W. Jin, L. Blum, J. Küpper and S. Trippel

145. 3D Electron Diffraction using MeV electrons at REGAE
A. C. Rodrigues, P. Reinke, M. Hachmann, M. Barthelmess, V. Hennicke, J. Meyer, W. Brehm, A. Tolstikova, L. de Melo Costa, S.T. Veedu, M. Galchenkova, O. Yefanov, H. Delsim-Hashemi, T. Pakendorf, L. Gumprecht, K. Flöttmann, H. Chapman and A. Meents

146. Characterization of variable polarization non-linear high order harmonic emission of a seeded free-electron laser and its application to time resolved spin dynamics at the L2,3 edge of magnetic transition metal.
F. Capotondi, M. Malvestuto, C. Spezzani, E. Allaria, L. Badano, A. Carretta, M.B. Danailov, D. De Angelis, A. Demidovich, G. De Ninno, B. Diviacco, D. Garzella, L. Giannessi, S. Laterza, M. Manfredda, I. Nikolov, M. Pasqualetto, M. Pancaldi, E. Pederesoli, G. Penco, G. Perosa, A. Ravindran, P. Rebernik, R.Richa, A. Simoncig, F. Sottocorona, S. Spampinati, F. Tripaldi, M.Trovò, M. Zangrando, R. Gruber, M. Klaui, S. Flewett, C. Mimming, J. Zhang, C. Léveillé, M. Sacchi and N. Jaouen

147. EuPRAXIA: The Path to Ultra-Compact Plasma Acceleration Users' Facilities
Z. Ebrahimpour on behalf of the EuPRAXIA_PP and LEAPS-INNOV projects' collaboration

148. NMRCoRe - a convergence research node with focus on molecular water science
E. Breynaert

149. New Developments in Diffractive X-ray Optics
A. Kubec, C. David, D. Eschimese, T. Mamyrbayev, J. Erjawetz and F. Döring

150. Compact RF gun setup for Ultrafast Electron Diffraction
G.H. Kassier, R. Bazrafshan, M. Fakhari, A. Özmat, H. Delsim Hashemi, T. Rohwer, K. Flöttmann, N. H. Matlis and F. X. Kärtner

151. High-energy and high-power cryogenic lasers for photon science facilities and advanced lasers for THz generation and pump-probe experiments
M. Pergament, M. Kellert, J. Thesinga, A. Yakovlev, M. Kilinc, U. Demirbas, S. Malekmohamadi and F. X. Kärtner

152. Training of Neural Networks for the Analysis of Grazing-Incidence X-ray Scattering Data
J. E. Heger and P. Müller-Buschbaum

153. Time-dependent Density Functional Theory for Matter under Extreme Conditions
K. Ramakrishna and A. Cangi

154. Charge Transfer in Ternary Quantum Dot Sensitized TiO_2 for Photocatalysis Studied by Ambient Pressure Time-Resolved XPS
M. Stapf, D. Potorochin, Z. Donnellan, S. D. Perera, O. Gessner, Y. Joseph, S. Molodtsov and F. Roth

155. X-RAYS meet NEUTRONS meet IONS meet ELECTRONS meet LASERS meet MAGNETS: combined access to multiple facilities through EU project ReMade@ARI
M. Stuckelberger, C. Ossig, G. Fevola, B. Schramm and S. Facsko

156. High-resolution X-ray diffraction study of (001)-oriented SnTe and Pb1-xSnxTe layers and MBE-grown on commercial GaAs substrate
A. Sulich, K. Dybko, W. Wołkanowicz, E. Łusakowska, P. Dziawa, J. Sadowski, B. Taliashvili, T. Wojtowicz, T. Story and J. Z. Domagala

157. The EuPRAXIA@SPARC_LAB FEL photon science plan
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158. Coded-Apertures for Depth-Resolved X-ray Laue Microdiffraction
D. Sheyfer, D. Gursoy, M. Wojcik, W. Liu, M. Prince and J. Tischler

159. Laser-driven and high-brightness THz and electron sources for photon science
N. H. Matlis, M. Pergament, T. Rohwer, T. Kroh, K. Ravi, R. Bazrafshan, M. Fakhari, G. Cirmi, H. T. Olgun, W. Tian, C. Rentschler, H. Çankaya, A.-L. Calendron, M. Vahdani, F. Ritzkowsky, T. Tilp, A. Berg, Z. Zhang, D. Zhang, H. Dinter, M. Kellermeier, Ü. Demirbas, J. Thesinga, S. Reuter, M. Kellert, R. Aßmann, T. Vinatier, G. Vashchenko, L. Zapata, M. Hemmer, F. Lemery, A. Fallahi and F. X. Kärtner

160. Advanced X-ray Polarimetry for the Detection of Vacuum Birefringence
W. Hippler, R. Lötzsch, K.-S. Schulze, B. Marx-Glowna, I. Uschmann and G. G. Paulus

161. Modulation of LCST behavior of thermo-responsive polymer by photo-responsive azo functionalities for schizophrenic switching
P. Zhang, R. Steinbrecher, A. Laschewsky, P. Müller-Buschbaum and C. Papadakis

162. FemtoMAX beamline: an instrument for femtosecond time-resolved x-ray diffraction/scattering and absorption spectroscopy
V.-T. Pham, B.-N. Ahn, D. Kroon, C. Ekström, A. Jurgilaitis, J. Larsson, J. Uhlig, C. Bressler, K. Kubicek, M. Sekkal, Z. Nurekeyev, A. Eriksson and H. Hwang

163. Exploring fingerprints of ultrafast structural dynamics in molecular solutions with an XFEL
R.P. Kurta, T.B. van Driel, A.O. Dohn, T.B. Berberich, S. Nelson, I.A. Zaluzhnyy, N. Mukharamova, D. Lapkin, D.B. Zederkof, M. Seaberg, K.S. Pedersen, K.S. Kjær, G.I. Rippy, E. Biasin, K.B. Møller, L. Gelisio, K. Haldrup, I.A. Vartanyants and M.M. Nielsen

164. Simulation and Design of a Novel Detector for Angular Streaking at FELs
L. Wülfing, A. Held, N. Wieland, L. Funke, S. Savio, M. Ilchen and W. Helml

165. Nanoscale structural dynamics by EUV transient gratings
F. Bencivenga, L. Foglia, C. Masciovecchio and R. Mincigrucci

166. Probing the Surface Polarization of Ferroelectric Thin Films by X-ray Standing Waves
L. P. Hoang, I. Spasojevic, T. L. Lee, D. Pesquera, K. Rossnagel, J. Zegenhagen, G. Catalan, I. A. Vartanyants, A. Scherz and G. Mercurio

167. Insights into the stratum Corneum Lipid Organisation in an Epidermal Cell Culture Model by Means of SAXS
J Kuntsche, S. Funari and P. Garidel

168. Exploring the Response of Liquids to Ionizing Radiation with Ultrafast X-rays and Simulations.
L. Inhester

169. Nanoscale X-ray imaging with high spectral sensitivity using incoherent diffractive imaging
T. Wollweber and K. Ayyer

170. Initiating and unravelling gas-phase thermal-energy dynamics.
M. S. Robinson, M. Singh, H. Bromberger, S. Trippel and J. Küpper

171. High repetition rate ultrafast electron diffraction with direct electron detection
F. Rodriguez Diaz, M. Meroe and K. Amini

172. 3D structure determination with accelerator based electron diffraction
P. Y. Reinke, V. Hennicke, M. Hachmann, J. Meyer, O. Yefanov, S. T. Veedu, A. C. Rodrigues, H. Hashemi, K. Flöttmann and A. Meents

173. Time-dependent Resonant Inelastic Scattering of Pyrazine at the Nitrogen K-edge: A Quantum Dynamics Approach
A. Freibert, D. Mendive-Tapia, N. Huse and O. Vendrell

174. Sarcomere and troponin and myosin X-ray diffraction signals can be resolved in single cardiomyocytes
H. Bruns, T. S. Czajka, M. Sztucki, S. Brandenburg and T. Salditt

175. Opportunities for ultrafast electron diffraction (UED) experiments at REGAE
A. Meents, V. Hennicke, M. Hachmann, T. Pakendorf, J. Meyer, P.Y.A. Reinke, O. Yefanov, S. Thekku Veedu, A.C. Rodrigues, A. Qelaj, H. Hashemi and K. Flöttmann

176. Revealing and Reading Cuneiform Scripts using Portable High-Resolution Computed Tomography
S. Ehteram, A. Schropp, C. Michel, R. Döhrmann, P. Wiljes, A. Becker, P. Paetzold, C. Waerzeggers, S. Olbrich and C. Schroer

177. DEMIST “Dual-Events Momentum Imaging Spectroscopy Tool”
T. Mazza, S. Sasikumar, S. Dold, M. Devetta, M. Coreno, S. Riboldi and P.Piseri

178. GPU-accelerated seed-skewness algorithm for rapid assessment of differential signal in time-resolved structural X-ray studies of metastable states
P. Łaski, D. Szarejko, R. Kamiński, K and Jarzembska

179. Liquid jet development at FERMI
M. Krstulovic, G. Bonano, M. Zamolo, A. Gessini, M. Coreno, E. Principi and R. Mincigrucci

180. Theoretical approach to polaritonic signatures in XPDC
F. Kerker, T. Quast, C. Boemer and D. Krebs

181. Investigation of the stability of oceanic sediments under hydrous cold subduction conditions
S. Yun and Y. Lee

182. Hydration breakdown of serpentines along cold core geotherm
H. Sim, Y. Bang, HP. Liermann, H. Hwang, N. Giordano, D. Zhang, P. Nguyen and Y. Lee

183. Computing ground and excited states of molecules with neural networks
Y. Saleh, A. Fernández, A. Iske, J. Küpper and A. Yachmenev

184. Attosecond insights into liquid systems
S. Bhattacharyya, L. Inhester, S. Li, L. Lu, C. I. Pearce, K. Li, E. T. Nienhuis, G. Doumy, R.D. Schaller, S. Moeller, M.-F. Lin, G. Dakovski, D.J. Hoffman, D. Garratt, K. A. Larsen, J.D. Koralek, C.Y. Hampton, D. Cesar, J. Duris, Z. Zhang, N. Sudar, J. P. Cryan, A. Marinelli, X. Li, L. Young and R. Santra

185. UV-induced chemical dynamics of solvated (bio)molecular complex system
M. Singh, M. S. Robinson, H. Bromberger, S. Trippel and J. Kuepper

186. Nexus - The Nuclear Elastic X-ray scattering Universal Software
L. Bocklage

187. Grazing Incidence X-ray Ptychography: Ultra high surface sensitivity with large field of view
L. Besley, P. S. Jørgensen, A. M. Slyamov, A. Diaz, M. Guizar-Sicairos, M. Odstrčil, M. Holler, C. Silvestre, B. Chang, C. Detlefs and J. W. Andreasen

188. Dynamic convergent shock compression initiated by return current in high-intensity laser solid interactions
L. Yang, L. Huang, M. Rehwald, T. Kluge, A. Laso, T. Toncian, K. Zeil, U. Schramm and T. E Cowan

189. Cellulose-based curtain integrated with non- fullerene organic solar cell
X. Jiang, Y. Guo, Z. Chen, M. Betker, D. Söderberg, N. Kölpin, P. Müller-Buschbaum, A. Willner and S. V. Roth

190. Tracking the Photoexcited Intramolecular Energy and Charge Transfer in a Small Push-Pull Type donor-acceptor molecular dyad
S. Manikandan, A.K. Schnack-Petersen, S. Coriani, K.B. Møller, C. Bacellar, C. Cirelli, M. M. Nielsen, K. Haldrup and J.W. Andreasen

191. Simulating Materials at High-Pressure with Ephemeral Data Derived Potentials
P. Cooke, P. Salzbrenner, L. Conway, C. Witt, S.H. Joo and C. Pickard

192. Centre for Molecular Water Science
C. Goy, S. Bari, E. Gougoula, F. Lehmkühler and M. Schnell

193. Investigation on x-ray radiation from microstructured targets heated by short-pulse relativistic laser pulses
X. Pan, M. Šmíd, L. G. Huang, V. Bagnoud, E. Brambrink, T. E. Cowan, J. Colgan, T. Ebert, D. Hartnagel, M. Hesse, J. Hornung, A. Kleinschmidt, P. Perez-Martin, A. Neukirch, K. Philipp, S. Sander, G. Schaumann, A. Tebartz, B. Zielbauer, M. Roth and K. Falk

194. Wakefield Plasma Lens and Ensuring a Reduction in Energy Spread for Gaussian-kind Bunches
I.V. Demydenko, V.I. Maslov, W. Leemans and M. Thevenet

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195. Towards high-throughput bio-medical tomography at GINIX II / PETRA IV
M. Osterhoff, B. Hartmann, F. Westermeier, M. Sprung and T. Salditt

196. Single shot reflectivity measurement at the Langmuir trough GID setup at beamline P08 of PETRA III
C. Shen, R. Kirchhof, B. Bharatiya and F. Bertram

197. Advancing the Fundamental Understanding of Novel Superalloys through Neutron and Synchrotron Radiation Studies
S. Neumeier, O. Nagel, J. Bandorf, A. Stark, F. Pyczak, C. Solis, M. Fritton, A. Mutschke, R. Gilles and M. Göken

198. Real-time data processing for serial X-ray crystallography
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199. Magnetometry of Buried Co-based Nanolayers by Hard X-ray Photoelectron Spectroscopy
A. Hloskovsky, Ch. Schlueter and G. Fecher

200. Evolution of morphology and optical properties of thin films probed in situ during spraying for organic solar cells
S. Xiong, B. Sochor, C. Harder, P. Müller-Buschbaum and S. V. Roth

201. Study on Structure and Dynamics and Functional Dysregulation of Bacterial Caseinolytic Protease P (ClpP) from Nosocomial Pathogen
B. Alves França, H. Rohde and C. Betzel

202. Development of the Continuous Readout Digitising Imager Array detector
A. Marras, A. Klujev, S. Lange, T. Laurus, D. Pennicard, U. Trunk, C.B. Wunderer, S. Spannagel, T. Vanat, H. Krueger and H. Graafsma

203. Revealing the Packing Behaviour of Au Nanocrystals in Mesocrystals using Angular X-ray Cross-Correlation Analysis
K. Hoon Ngoi, D. Lapkin, G. Hinsley, S. Sturm, R. Rysov, F. Kirner, S. Singh, D. Assalauova, M. Sprung, E. Sturm and I. A. Vartaniants

204. In-situ synthesis of Au@FeOx nanoparticles using SAXS/WAXS
X.Sun and J.Zhang

205. PETRA III: Advanced Applications of Synchrotron Radiation.
O. Seeck, H.-C. Wille and C. Schroer

206. Compton microscopy with multilayer Laue lenses
S. Bajt, T. Li, M. Prasciolu, N. Ivanov, H. Fleckenstein, O. Yefanov, W. Zhang, D. Pennicard, A.-C. Dippel, O. Gutowski, P. Villanueva-Perez and H. N. Chapman

207. An ML-driven XANES interpretation for nanocrystal determination in operando catalysis.
A. Sapronov, D. Doronkin, A. Zimina and J.D. Grunwaldt

208. In-operando studies of piezoelectric $HfZrO_2$ on III-V semiconductor nanostructured
S. Singh, N. Zaiats, Z. Ren, R. Rysov, M. Sprung, A. Mikkelsen and I. A. Vartanyants,

209. P61B LVP: In situ high-pressure studies using white beam in the Large Volume Press
R. Farla, S. Bhat, K. Spektor, C. Lathe, S. Ma, A. Neri, L. Man, A. Chanyshev, S. Sonntag, U. Haeussermann and T. Katsura

210. Bridging the Timescales Between Coherent Diffractive Imaging and X-ray Photon Correlation Spectroscopy
G. Hinsley, F. Westermeier, R. Rysov, K. H. Ngoi, B. Wang, S. Singh, M. Sprung, C. Kewish, G. van Riessen and I. Vartaniants

211. Unique experimental setups for in situ characterization of structure formation in polymer materials
E. Euchler, A. K. Sambale, R. Boldt, K. Uhlig, K. Schneider, M. Schwartzkopf, S.V. Roth and M. Stommel

212. The chemical crystallography beamline P24
M. Tolkiehn, L. Noohinejad, P. Pokhriyal, C. Paulmann and H. Schulz-Ritter

213. Small and Wide Angle X-ray Scattering imaging capabilities at the SAXSMAT beamline.
A. L. C. Conceicao, S. Pfeffer and S. Haas

214. Thickness-dependent efficiency of fully sprayed organic thin film thermoelectrics
B. Sochor, S. Schraad, L. Huber, A. Hexemer, T. Laarmann, S. K. Vayalil, P. Müller-Buschbaum and S. V. Roth

215. Structure and Dynamics of the Penicillin-binding Protein 3 from Staphylococcus epidermidis native and in Complex with Cefotaxime and Vaborbactam
M. Schwinzer, H. Brognaro, H. Rohde and C. Betzel

216. Full field micro tomography at beamline P05
J. U. Hammel, F. Beckmann, J. Moosmann, L. Lottermoser, O. Lippmann, H. Burmester, J. Brehling, U. Tiezte, B. Schwebke and F. Wilde

217. Adsorption of cysteine in the surface of titania
M. Blanco Garcia, M. Kohantorabi, M.Wagstaffe, A. Stierle and H. Noei

218. First x-ray measurements with the TEMPUS system at PETRA III
J. Correa, D. Pennicard, S. Fridman, S. Lange, H. Graafsma, H. Bromberger, A. Samartsev, I, Sergeev, D. Prajapat, S. Velten, L. Merten Lohse, A. Ignatenko, R. Roehlsberger, B. Senfftleben, S. Karl and J. von Zanthier

219. In-situ SAXS Study of the Facile Assembly of Au-Fe_3O_4 Heteronanoparticles
J. Zhang, X. Liu, F. Bertram, C. Shen, W. J. Parak and X. Sun

220. Injectable hydrogels from thermoresponsive tri- and tetrablock terpolymers investigated using scattering methods
F. Zheng, P. A. Álvarez Herrera, W.Xu, E. Melampianaki, A. Constantinou, L. Wang, T. K. Georgiou and S. Da Vela

221. Comparison of dcMS and HiPIMS Gold Deposition on Polystyrene and Poly-4-vinylpyridine and Polystyrenesulfonicacid
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223. Multibeam Ptychography: like a single beam but way faster
M. Lyubomirskiy, T. Li, M. Kahnt, T. L. Sheppard, R. Yang, K. Vidar Falch, R. Zvagelsky, P. Villanueva-Perez and M. Wegener

224. Quantitative Phase-contrast Microtomography at Beamlines P05 and P07 (PETRA III)
D. John, M. Riedel, A. Gustschin, M. Busse, L. Petzold, N. Pellegata, F. De Marco, P. Thibault, F. Beckmann, J. Moosmann, J. Hammel and J. Herzen

225. Ultra-lightweight compositionally complex alloys with large ambient-temperature hydrogen storage capacity
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A worldwide voice for the light source user community


DESY
Campus in Hamburg-Bahrenfeld
Location Users' meeting
'Kuppel Hamburg'
Luruper Chaussee 30
22761 Hamburg
Side gate
Main gate
DESY guest house
Luruper Chaussee/DESY
Bus 2, 3, X3, 284
Trabrennbahn
Bahrenfeld
Luruper Chaussee
Notkestraße
Ebertallee
Hamburg City
Bertr.-Russel-Straße
Albert-
Einstein-
Ring
Max-Born-Straße
European XFEL
CSSB
AER19
AER17
Footpath to Footpath to Users'meeting
(Trabrennbahn)