FELs OF EUROPE NEWS 1|20

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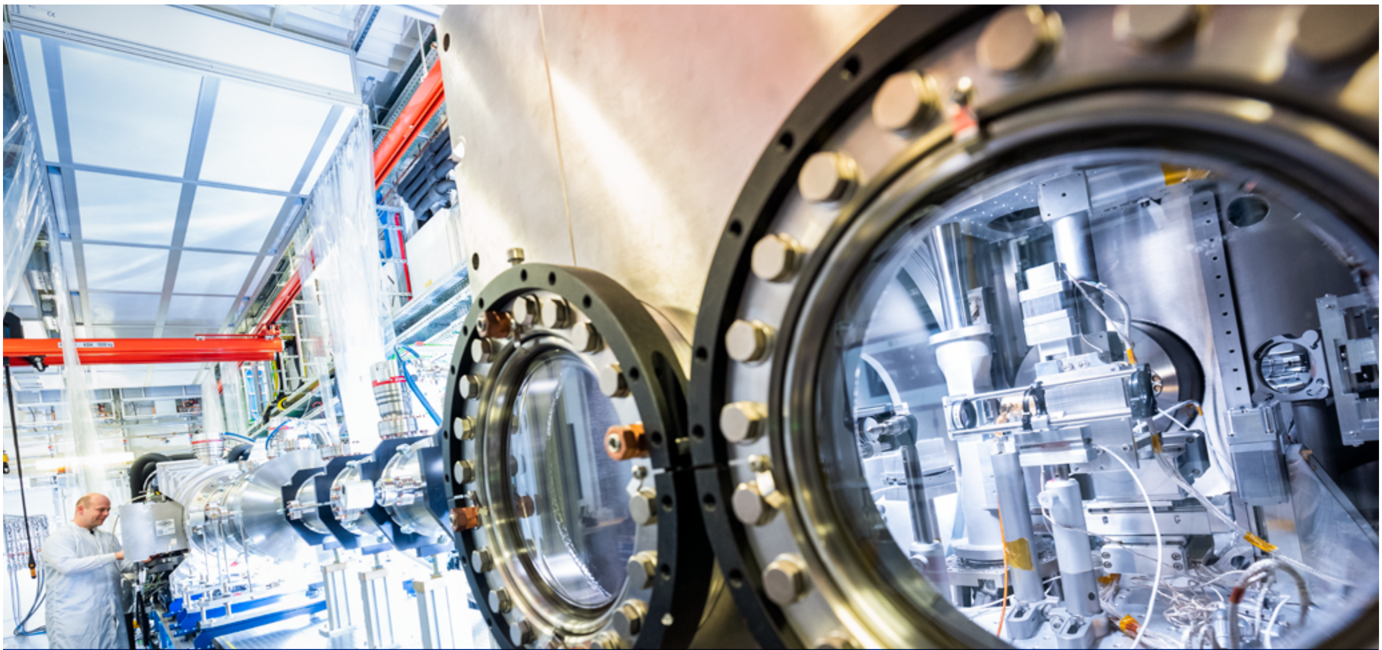

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FELs OF EUROPE is pleased to present the first 2020 issue of the Newsletter. The situation with the COVID-19 pandemic has impacted the operation of our facilities and difficulties have been encountered especially during the first phases of the crisis. However, the accelerator-based light sources have proven to adapt the way of operation very swiftly and several facilities within our collaboration have opened in March already calls for rapid access to dedicated beamtime on the SARSCoV-2 virus. The retarded publication of this issue gives us the opportunity to report on several contributions about the research performed at our facilities on the SARSCoV-2 virus. The experience over the last months showcases the importance of keeping our facilities fully operational during complex crisis periods; a key challenge for the future is to make the FELs and the photon sources in general more resilient. This challenge is already taken up by the LEAPS collaboration that intends to jointly work towards a "Digital LEAPS".

This Newsletter moreover includes then a number of research highlights that once more are showing the high level of the scientific activities that are run at the FEL facilities in Europe. Further opportunities to share most recent scientific findings and results at our facilities will be at the two upcoming events organized by FELs OF EUROPE, i.e. the SCIENCE@FELs 2020 conference, originally scheduled in September in Hamburg at DESY and European XFEL, and the PhotonDiag 2020 workshop, originally scheduled in October at PSI. Both events will now be conducted in a fully online format, as a result of the pandemic situation.

We hope you will enjoy reading the new issue of the FELs OF EUROPE Newsletter. Looking forward to meeting again in person soon, keep safe and stay healthy!

Michele Svandrlik

FELs OF EUROPE

COVID-19 related activities

Europe's Accelerator-Based Photon Sources join forces in fighting COVID-19

LEAPS

LEAPS facilities are joining forces in front of the coronavirus pandemic, offering their capacities to the whole scientific community. Several facilities have opened calls for rapid access to dedicated beamtime for prioritizing the research on the SARSCoV-2 virus, its therapy and vaccine, above the rest, aiming at minimizing the time from proposal to paper submissions.
An overview of participating facilities is available on the LEAPS website: https://leaps-initiative.eu/leaps-facilities-research-on-sars-cov-2/ Moreover, LEAPS published a paper and sections A to G summarize the LEAPS instrumentations and methods that are at the service of the world scientific community. Examples of the first results, which are being obtained and publicly available, are also shown. Boosting the existing capacities with adequate national and European funding programs, will place the LEAPS consortium in a privileged position to be one of the mayor players for addressing the present and future viral threats the society is facing. For further information the paper can be downloaded here https://leaps-initiative.eu/wp-content/uploads/2020/05/LEAPS_fighting_COVID19_May2020.pdf

Britta Redlich

European XFEL open for COVID-19 research

European XFEL

European XFEL will contribute to the global research effort investigating the novel Coronavirus, SARS-CoV-2. After six weeks in reduced operation mode, European XFEL restarted operation of the X-ray laser on 4 May. Regular user operation is not possible yet, however, the facility is accepting proposals for COVID-19 related research at the instruments and research laboratories.

One of the six European XFEL experiment stations, the SPB/SFX instrument, is dedicated to structural biology applications. Several features of the facility make it particularly well suited to this research. Structural biology experiments can be performed at room temperature at XFELs, rather than at cryogenic temperatures as is typical at synchrotron light sources. This would enable complexes of interest, such as a protein from SARS-CoV-2 with a drug candidate bound to it, and which have been previously identified at synchrotron sources to be examined at near-physiological temperatures. In addition researchers may be able to observe the dynamics of biological reactions and processes such as the interaction between viral and host proteins. European XFEL provides comprehensive support to visiting scientists in sample delivery to the X-ray beam and data analysis.
Even before the reopening of beamlines, researchers at European XFEL's user-consortium supported biology laboratory XBI, together with researchers from DESY and other institutions, are engaged in screening for SARS-CoV-2 antiviral drugs as well as contributing to research on viral assembly and the structure and function of non-structural viral proteins.

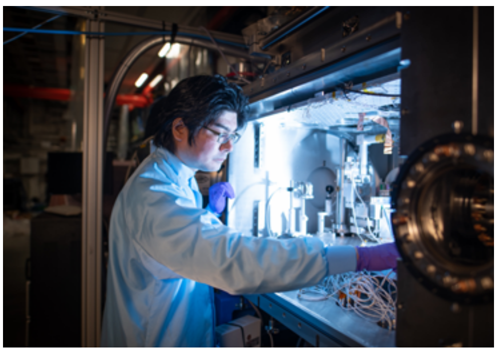
European XFEL scientific director Sakura Pascarelli: "We hope that the research we plan to do will enable rational drug design not just in the current crisis, but also with the long-term potential to better understand the processes of virus entry, replication and release in detail. We will intensify our collaborations with laboratories and the scientific community worldwide to be ready to address other, future urgent public health issues requiring rapid-response structural biology."

A broader framework for a coordinated research programme into COVID-19, including X-ray experiments as well as laboratory, sample environment and data analysis capacities, is currently being developed with the European XFEL user community and will be announced in the near future. At the same time European XFEL will upgrade experimental capabilities to better address this and future biological challenges.

To remain informed subscribe to the SPB/SFX mailing list.

Bernd Ebeling

The experiment station SPB/SFX is used to investigate the three-dimensional structures of biological objects including viruses. Copyright European XFEL / Jan Hosan



Scientist Tokushi Sato working at the sample chamber of the SPB/SFX instrument. Copyright European XFEL / Jan Hosan

Picture on the cover page:
Experiments at X-ray free-electron lasers (XFELs) can be performed at room temperature which is an advantage when observing the interaction between viral and host proteins. Copyright European XFEL / Jan Hosan

FERMI is carrying out experiments to elucidate the function of antiviral drugs

FERMI

The recent spread of COVID19 infection calls for concerted and rigorous effort of various specialists aimed at finding a cure to it, and in particular at finding drugs that minimize its effects. Among these drugs, the popular and water-soluble chloroquine (CQ (N4-(7-Chloro-4-quinolinyl)-N1,N1-diethyl-1,4-pentanediamine)) and its derivatives, hydroxychloroquine (HQ) and ferrocene-chloroquine (FQ) have emerged as potential cures against the disease. These have been used for decades as anti-malarial drugs but recent trials have shown that they could cure patients affected by the Covid-19. This makes it even more valuable given that presently, there are no commonly agreed on prophylactic or therapeutic treatment options for Covid-19 and a vaccine is not expected to be developed and available to the wider population for 12-18 months.

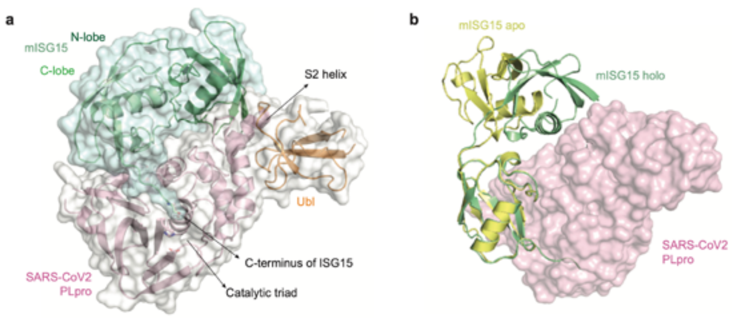
CQ and its derivatives act as weak bases, which preferentially accumulate within intracellular compartments (including endosomes, lysosomes, and Golgi vesicles). CQ has multiple activities, one of which is to increase the pH of intracellular vesicles as mentioned earlier, interfering with the pH-dependent steps of viral replication, including fusion and uncoating. It is believed that lysosomotropic agents (of which CQ is included) can effectively inhibit coronavirus as the latter requires acidification of endosomes for proper functioning. However, the action mechanism of the CQ class remain unclear, especially at the molecular level. A recent study has shown its capacity to play a role in mechanisms, which involve the virus spike envelope glycoprotein (S) and the Angiotensin converting enzyme 2 (ACE2) located on the cellular membrane. The interaction between these two macromolecules triggers the fusion between the virus and the host cell initiating the invasion. These various findings suggest that CQ and its derivatives first interact with the cellular membrane, but how this takes place is wholly unknown to date. A study is going to be carried out at FERMI with the aim to specifically address this issue by investigating the molecular level interaction of CQ and its derivatives with the cellular membranes. The capability of FERMI to access low frequency vibration, responsible for the bio-activity of pharmaceutical compounds, with atomic and enantiomeric sensitivity, allows, in principle to understand how chloroquine interacts with ligands. This study is a collaboration among different institutions: EPFL, University of Irvine, University of Bologna and Elettra Sincrotrone Trieste.

Claudio Masciovecchio

First PSI MX results of the priority COVID-19 call

PSI

PSI has opened a 'PRIORITY COVID-19 Call' for short proposals and quick peer review to enable rapid access to beamtime. Scientists from the Goethe University in Frankfurt am Main, Germany have published results on the papain-like protease (PLpro), an essential enzyme of SARS-CoV-2. The structural biology work was performed at the macromolecular crystallography beamline X06SA-PXI at SLS following the opening of the "PRIORITY COVID-19 Call". The paper was submitted within one month after answering the proposal call. The crystallographic data collection happened on the 9th of April after the planned Easter shutdown of the SLS was cancelled for this specific experiment. The protease PLpro is required for the processing of viral polypeptides and the assembly of new viral particles within human cells. In addition, SARS-CoV-2 uses this enzyme to dampen the anti-viral immune response, helping the virus to modulate the host's immune system to its own benefit. By this, the virus can easily multiply and spread further. The team has demonstrated that pharmaceutical targeting of PLpro by a non-covalent inhibitor (GRL-0617) blocks virus spread and increases anti-viral immunity in human epithelial cells, the prime site of pathogen entry. The respective results were made publicly available on a preprint server https://www.researchsquare.com/article/rs-27134/v1. The PDB 6YVA https://www.rcsb.org/structure/6YVA was released on the 13th of May.



Structural analysis of SARS-CoV-2 PLpro in complex with full length ISG15

Publication:

Inhibition of papain-like protease PLpro blocks SARS-CoV-2 spread and promotes anti-viral immunity, http://doi.org/10.21203/rs.3.rs-27134/v1

Call:

https://www.psi.ch/en/macromolecular-crystallography/scientific-highlights/first-mx-results-of-the-priority-covid-19-call

Contact:

Dr. Vincent Olieric, Swiss Light Source e-mail: vincent.olieric@psi.ch
Dr. Meitian Wang, Swiss Light Source e-mail: meitian.wang@psi.ch

FELS OF EUROPE: RAPID ACCESS COVID-19

Research on the SARS-CoV-2 virus, which causes the current outbreak of COVID-19, is a global endeavor. Several facilities within our collaboration have started research on SARS-CoV-2 virus and opened calls for rapid access to dedicated beamtime.

European XFEL call for expressions of interest in COVID-19 related research
https://www.xfel.eu/index_eng.html

FELIX in the Netherlands offers rapid access route:
https://www.ru.nl/felix/vm/rapid-access-corona-related-research-felix/

MAX IV Laboratory in Sweden provides rapid access:
https://www.maxiv.lu.se/news/rapid-access-call-for-proposals-sars-cov-2-and-urgent-e-g-health-related-research/

Soleil in France provides rapid access:
https://www.synchrotron-soleil.fr/en/news/covid-19-research-synchrotron-soleil-and-rapid-access

DESY in Germany offers rapid access to PETRA III beamlines:
https://photon-science.desy.de/users_area/fast_track_access_for_covid_19/index_eng.html

BESSY II at HZB in Germany provides fast track access to their instruments for issues of highest relevance:
https://www.helmholtz-berlin.de/forschung/oe/np/gmx/index_en.html
Contact: Manfred Weiss, team leader of MX joint research group

Swiss Light Source and Swiss FEL at PSI in Switzerland offer priority access to combating COVID-19:
https://www.psi.ch/en/psd/covid-19

Elettra Sincrotrone Trieste in Italy opens to remote access following beamlines: XRD1, XRD2, SISSI-BIO and MCX:
https://www.elettra.trieste.it/userarea/covid-19-virus-elettra-rapid-access-proposals.html

For an overview of all facilities of the LEAPS collaboration offering rapid access:
https://leaps-initiative.eu/leaps-facilities-research-on-sars-cov-2/

LEAPS facilities join forces in fighting COVID-19
https://leaps-initiative.eu/wp-content/uploads/2020/05/LEAPS_fighting_COVID19_May2020.pdf

Summary of FELs OF EUROPE (FOE) Activities 2019

Core activities

- 3 Face-To-Face meetings, at HZB Berlin in March, at the FEL 19 conference in Hamburg in August and at PSI in November 2019
- New P&R material as memory sticks, with the FOE Whitebook uploaded, ball pens, postcards and a printed version of the FOE newsletter 1/19 have been produced
- Website updated and maintained (https://www.fels-of-europe.eu)
- The activities of the FOE expert working groups (seeding, photon pulse length measurement, instrumentation) have been revised and a reorganization will be pursed, with the goal to focus on those aspects of interest of all partners of FOE, in particular those not part of LEAPS.
- July and December issues of the FOE Newsletter published

Events and Dissemination

- FOE booth with an information point at the FEL 19 Conference in Hamburg (26-30 August). It was well attended by the conference delegates and it resulted very important for the visibility of the collaboration and for spreading the knowledge about its activities.
- Guidelines for the future organizers of FOE events have been provided, to ensure uniform organization of the upcoming events.
- Organization of the SCIENCE@FELs Conference 2020 (14-17 September, Hamburg, DESY and European XFEL) started
- Forum on Advanced FEL Techniques, approved again as a satellite event to the SCIENCE@FELs 2020

FELs OF EUROPE

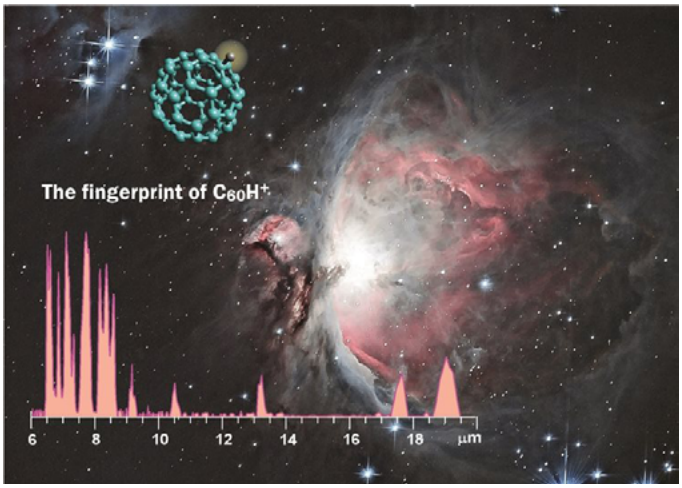
The IR spectrum of protonated buckminsterfullerene $C_{60}H^+$

FELIX Laboratory

Although fullerenes have long been hypothesized to occur in interstellar environments, their actual unambiguous spectroscopic identification is of more recent date. C_{60}, C_{70} and C_{60}^+ now constitute the largest molecular species individually identified in the interstellar medium. FELIX researchers have recorded the first laboratory IR spectrum of gaseous $C_{60}H^+$.

Fullerenes have significant proton affinities and it was Sir Harold Kroto who suggested that $C_{60}H^+$ is likely the most abundant interstellar analogue of C_{60}. To record the first laboratory infrared (IR) spectrum of $C_{60}H^+$ in the gas phase via infrared multiple-photon dissociation, FELIX researchers used the free-electron laser and an ion trap mass spectrometer. The added proton breaks the high symmetry of C_{60} producing a much richer IR spectrum, forming a textbook example of the influence of molecular symmetry on IR spectroscopy. The experimental spectrum is used to benchmark theoretical spectra indicating that the B3LYP density functional with the 6-311+G(d,p) basis set reproduces the spectrum most closely. Moreover, and perhaps most interesting, comparison with astronomical spectra from two planetary nebulae that have been associated with high abundances of neutral C_{60} indicate that $C_{60}H^+$ is a plausible contributor to their IR emission, possibly confirming Kroto's hypothesis.

Jos Oomens



The laboratory IR spectrum of $C_{60}H^+$. The background shows the Orion Nebula.

Original publication:
Julianna Palotás, Jonathan Martens, Giel Berden and Jos Oomens,
The infrared spectrum of protonated buckminsterfullerene $C_{60}H^+$
Nature Astronomy 4, 240-245 (2020)
https://doi.org/10.1038/s41550-019-0941-6

Big Data at FELs: Retrieving the shapes of spinning superfluid droplets with the help of a deep neural network for automated image recognition

FERMI

In a collaborative experiment at the FERMI free-electron laser, scientists were able to collect tens of thousands of single-shot coherent diffraction images (CDI) of nanometer-sized superfluid helium droplets and retrieve the droplets' three-dimensional (3D) shapes and orientations [Langbehn2018]. By training a residual neural network that was optimized for the application to coherent diffraction images, they could sort the huge data set into different classes [Zimmermann2019], making it thus analyzable.

3D shapes of spinning helium droplets

The approach enabled the team to address the question of which forms liquid rotating droplets take on in the absence of friction. The deformation of droplets from classical fluids under rotation is well researched and used to describe many objects in nature, from stellar bodies (the earth is for example a rotating liquid drop with a slightly oblate shape) to deformed atomic nuclei. While a resting droplet is of course spherical, with increasing angular velocity a spinning droplet becomes more and more oblate, before it transforms into a prolate, then even two-lobed shape and ultimately fissions into two drops. In a superfluid droplet, however, the atoms experience no friction. Angular momentum therefore leads to the formation of vortices that store the rotational energy. One could imagine that, in consequence, superfluid droplet shapes might differ from those of classical liquids. Indeed, in a first study on helium nanodroplets using hard X-ray diffraction, indications of extremely flattened oblate forms were found [Gomez2014], an unstable configuration for drops of classical liquids. In the X-ray spectral range, however, scattering images can typically be recorded up to small angles and in consequence, only two-dimensional projections of the particle shapes can be obtained. From the projection alone, a distinction between certain prolate and extremely oblate forms cannot be made. In contrast, when recording the scattered light up to large angles, which is possible with the XUV wavelengths of the FERMI FEL, 3D information on the droplet shape is encoded in the scattering patterns. For certain droplet orientations this manifests in pronounced asymmetric features in the diffraction pattern (see Fig 1 a for experimental and b for simulated pattern of a prolate droplet). This enables a unique 3D shape retrieval procedure and a comparison to calculated shapes of rotating drops (Fig. 1c). The researchers found that regarding the evolution of the shapes, superfluid droplets closely follow their normal liquid counterparts. In addition to this surprising result, no indications for the previously reported extremely oblate droplets were observed.

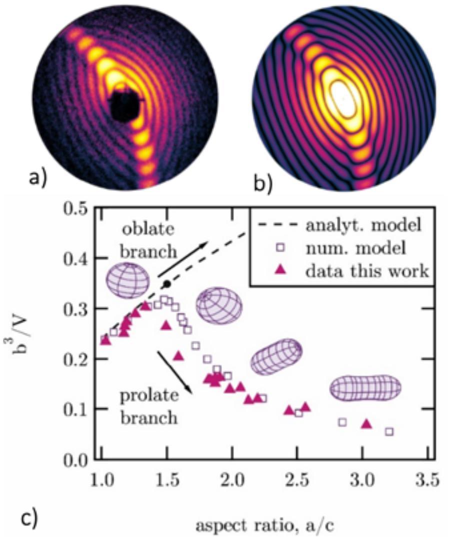


Fig 1: (a) Experimental and (b) simulated diffraction pattern of a prolate droplet. (c) Comparison to calculated shapes of rotating drops, expressed as a function of the principal semiaxis lengths a, b, c, and of the droplets' volume V. Adapted from B. Langbehn et al., "Three-Dimensional Shapes of Spinning Helium Nanodroplets" Phys. Rev. Lett. 121, 255301 (2018). DOI: 10.1103/PhysRevLett.121.255301 under the terms of the Creative Commons Attribution 4.0 International license.

Machine-learning-assisted coherent diffraction imaging

The large size of the data set obtained in this experiment with more than 40000 bright scattering patterns of individual droplets was necessary for a successful structure determination: a sufficient number of images that exhibit the characteristic asymmetries had to be present to identify all stages of the shape transition from oblate to prolate and two-lobed. At the same time, the huge quantity of images represents a significant problem for data analysis, and this problem is common to all coherent diffraction imaging approaches.To manually classify tens or even hundreds of thousands of individual patterns exceeds the capability of a human researcher, rendering the task of manually sorting data from tedious to impossible. Automated processes have to be developed, and today's state-of-the-art image recognition algorithms are readily available for this task. The researchers demonstrated in their seminal work [Zimmermann2019] that deep neural networks, when adapted to the domain of coherent diffraction imaging, can be used to classify large amounts of diffraction data. Therefore, a smaller and more manageable subset of the data has to be manually labeled by a researcher and is then used to train the network (see scheme of the training sequence in Fig. 2). The scientists systematically benchmarked their neural network approach and found that the trained neural network significantly outperforms previous attempts for automatically sorting and classifying complex diffraction patterns. The results demonstrate that the combination of high-quality FEL sources and automated data-mining approaches is opening up a new and exciting toolbox for studying the structure and dynamics of nanoscale objects with unprecedented precision.

Carlo Callegari, Daniela Rupp

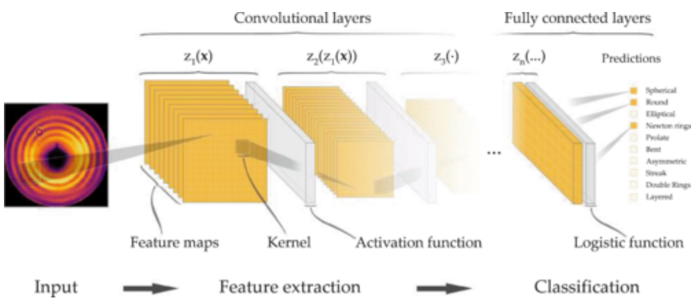


Fig 2: Schematic visualization of a convolutional neural network, trained to recognize features in coherent diffraction images. Adapted from J. Zimmermann et al., "Deep neural networks for classifying complex features in diffraction images" Phys. Rev. E 99, 063309 (2019). DOI: 10.1103/PhysRevE.99.063309 under the terms of the Creative Commons Attribution 4.0 International license.

Original publications:

[Langbehn2018] B. Langbehn *et al.*, "Three-Dimensional Shapes of Spinning Helium Nanodroplets", Phys. Rev. Lett. 121, 255301 (2018)
[Zimmermann2019] J. Zimmermann et al., "Deep neural networks for classifying complex features in diffraction images" Phys. Rev. E 99, 063309 (2019)

Additional references:

[Gomez2014] L. F. Gomez et al., Science 345, 906 (2014)

Study at FLASH - Polarization-sensitive reconstruction of THz fields at dielectric interfaces

The unique FLASH THz facility is worldwide leading in providing tunable narrowband Terahertz (THz) pulses with intrinsic synchronisation to soft X-ray pulses. These THz pulses are continuously tunable in the range of 10-300μm (4-125 meV) and the energy per pulse is in the range of several 100μJ for pump-probe experiments at the free-electron laser FLASH at DESY.

A group of scientists from University of Zurich, ETH Zurich, Paul Scherrer Institute (all from Switzerland), Universität Augsburg and DESY utilized this unique high-field THz accelerator-based radiation source to characterize the electric field of the THz pulse supposed to drive ultrafast processes at solid surfaces. This novel, in-situ approach is based on photoelectron streaking. This means that after the soft X-ray pulses from FLASH photoionized the sample the momentum distribution of the instantaneously created electrons was modified by the presence of the strong THz field.

Photoelectron streaking has been used in the past for pulse characterization. In this study, the authors take advantage of a 2D angle-resolved electron analyzer that gives access to the individual polarization components of the THz field. In addition, they directly probe the effective field at the surface. They noticed a substantial difference in the data coming from a bulk metal surface

and a nano-structured Pt thin-film, which can be related to the different screening behaviour of the materials. In this experiment they also used a back-reflecting multilayer mirror designed and prepared at DESY multilayer lab. This high reflectivity and narrow band mirror enabled to spatially overlap THz and soft X-ray pulses on the sample and to suppress unwanted background.
The development of a polarization-sensitive near-field probe with chemical sensitivity is of high interest for many fields (optoelectronics, nano-plasmonics) and this work paves the way for direct probing of near-field effects at nanostructures.

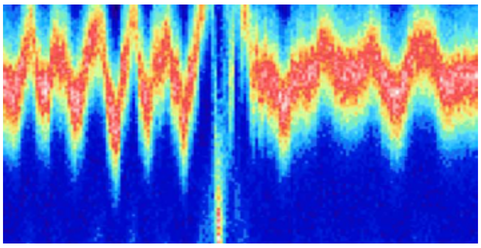


Fig 1: THz streaking of the Pt(111) valence level of the thin-film sample. A whole delay trace is shown in the figure below.
(Source: Original publication Optica 2019)

FLASH

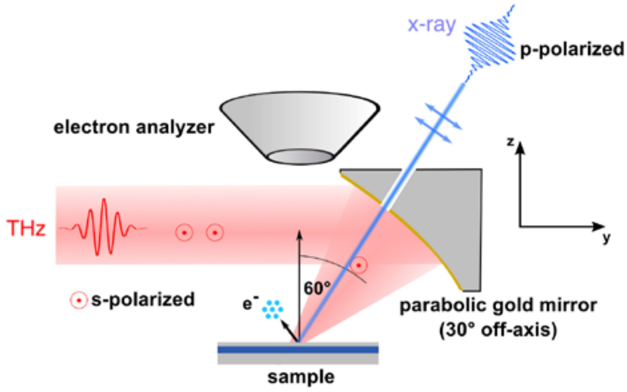


Fig 2: Angle-integrated delay trace of the thin film sample (top) and reconstructed field components parallel (center) and perpendicular (bottom) to the sample surface.
(Source: Original publication Optica 2019)

References:
Polarization-sensitive reconstruction of transient local THz fields at dielectric interfaces, K. Waltar, J. Haase, R. Pan, T. Golz, P. Kliuiev, M. Weinl, M. Schreck, S. Bajt, N. Stojanovic, J. A. van Bokhove, M. Hengsberger, J. Osterwalder, and L. Castiglioni, Optica 2019; DOI: 10.1364/OPTICA.6.001431

Laser plasma acceleration based tunable narrow bandwidth undulator radiation

SOLEIL

The laser discovery followed by the Free Electron Laser (FEL) invention led to the advent of X-ray FELs opening new areas for matter investigation with high temporal and spatial resolution. The parallel development of high accelerating gradient LPA [1] (0.1 – 10 GeV energy, kA peak current, ultra-short bunches, 1ϖmm. mrad normalized emittance beams) open hopes form them to drive undulator radiation and free electron lasers (FEL) light sources. Still, present LPA parameters (in particular the energy spread and the divergence [2]), do not meet conventional accelerator state-of-the-art performance, and require some electron beam manipulation along a transfer line. Proof-of-principle LPA based undulator emission, with strong electron focusing or transport, does not yet exhibit the full specific radiation properties. We report on the generation of undulator radiation with an LPA beam based manipulation in a dedicated transport line with versatile properties.

The LPA electrons are developed at Laboratoire d'Optique Appliquée (Salle Jaune) in the frame of an ERC Advanced Grant X-FIVE (PI V. Malka). A Ti:Sapphire laser system delivering 1.5 J, 30 fs FWHM pulses is focused into a supersonic jet of He-N2 gas mixture for a robust ionization injection, providing beams up to 250 MeV with a typical charge density of ~0.5 pC/MeV with few mrad divergence. The COXINEL manipulation line has been designed (see Fig. 1) and built [4] at Synchrotron SOLEIL in the frame of an ERC Advanced Grant COXINEL (PI M. E. Couprie) considering 200-400 MeV beams with 1 % energy spread, 1 mrad divergence, 1 Πm size and 4 kA peak current. It is installed at Laboratoire d'Optique Appliquée, where the LPA electrons are produced and accelerated. The divergence is rapidly mitigated via strong focusing with a triplet of so-called QUAPEVA adjustable permanent magnet quadrupoles [5]. A magnetic chicane then longitudinally stretches the beam, sorts electrons in energy and selects the energy range of interest via a removable and adjustable slit mounted in the middle of the chicane. A second set of quadrupoles matches the beam inside an in-the U18 cryo-ready undulator (107 x 18.16 mm period) [3]. The undulator radiation can be observed on a CCD camera and on a Horiba iHR320 spectrometer equipped with a CCD camera. The transverse pattern measured with a CCD camera is well reproduced by the simulations using measured electron beam characteristics for the transport along to the undulator to model the undulator radiation [6]. The spatio-spectral distribution of the UV light exhibits the typical "moon-shape" pattern resulting from the red shifted off-axis radiation (wavelength parabolic dependence with the observation angle), as confirmed by the different horizontal and vertical cuts [7].

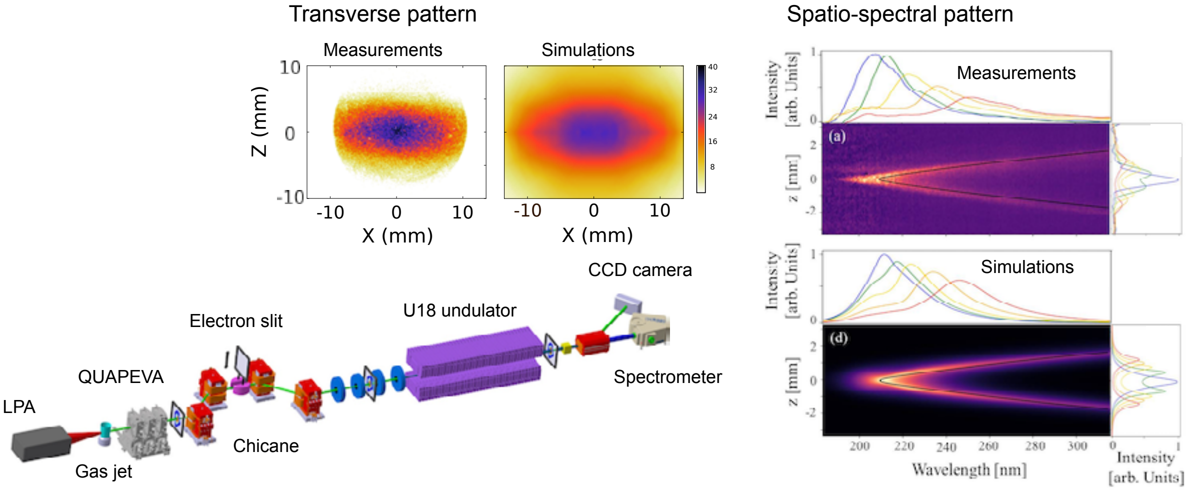


Fig. 1 : COXINEL line scheme. Transverse undulator radiation pattern measured with a CCD camera. Spatio-spectral pattern measured with a spectrometer equipped with a CCD camera in case of a 3 mm electron slit (3 % energy spread) at 5 mm gap with vertical positions at z = 0 (blue), 0.2 mm (green), 0.4 mm (yellow), 0.6 mm (orange), 0.8 mm (red) and vertical radiation profiles with cuts at different wavelengths 208 (blue), 228 (green), 248 (yellow), 268 (orange), 288 (red) nm. Black curve: fit of the undulator resonance wavelength cnsidering the chromatic aberrations of the lens. Comparisons with simulations using the electron beam measured parameters transported along the line show a good agreement.

The undulator resonant wavelength is then adjusted by varying the undulator gap [7], as illustrated in the measured spatio-spectral distributions in Fig. 2(a-d). The measured wavelength increases for gap closing for two electron beam energy settings, shown in Fig2(e) agrees with theoretical expectations from magnetic measurements. The resonant wavelength can thus be tuned within 200–300 nm by modification of the electron beam energy and the undulator field.

The undulator radiation spectral purity can also be controlled by adjusting the electron beam energy spread using the slit located in the chicane. The thickness of the moon shape patterns and the linewidths of the appended spectra shown in Fig. 3(a-d) decrease when the energy spread is reduced. The measured spectral purity improvement in Fig 3(e) for lower energy spreads follows the trend of the simplified analytic dependence and quantitatively agrees with the radiation modelling using electron beam properties in the undulator deduced from the measured ones transported along the line. The maximum calculated spectral brightness is found to be ~1 × 1018 ph/s/mm2/mrad2/0.1% BW.

Marie-Emmanuelle Couprie

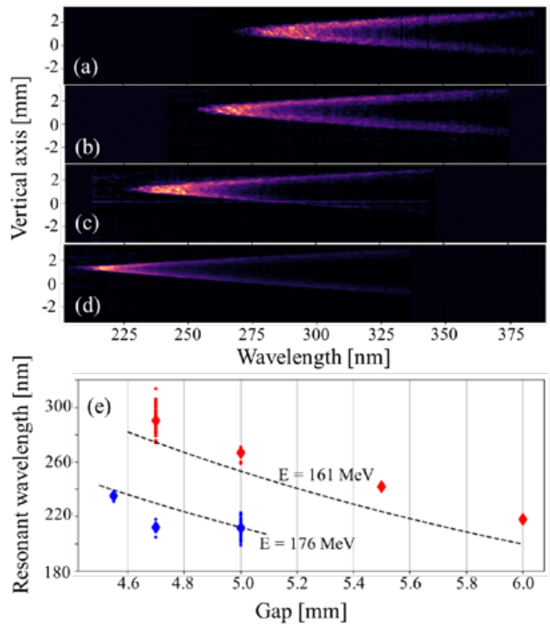


Fig. 2 : Single shot undulator spatio-spectra distribution measured for 161 MeV beam energy at different gaps: (a) 4.7 mm, (b) 5 mm, (c) 5.5 mm, (d) 6 mm, with an electron slit of 1 mm (energy spread of 1.4 %). (e) Measured and theoretical (dashed) resonant wavelength versus undulator gap: 161 MeV (red) and 176 MeV (blue).

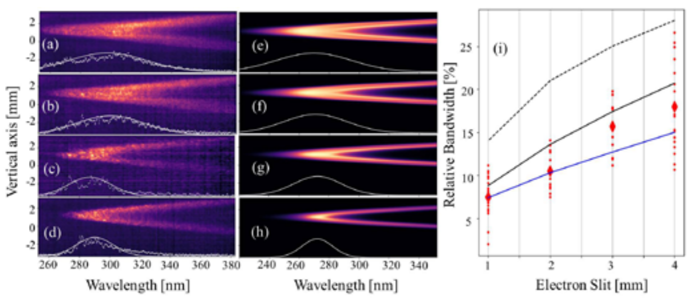


Fig. 3 : Measured single shot undulator spatio-spectral distributions (a, b, c, d) at 4.7 mm gap and simulated ones (e, f, g, h) using SRW for a magnetic field of 1.17 T, with beam parameters taken from the simulations of the corresponding electron beam distribution transported along the line versus energy spread: 3.1 (a, e), 2.6 (b, f), 2 (c, g) and 1.4 % (d, h). (i) Measured (red), analytically estimate of energy spread contribution (blue), analytically estimate of all the contributions (dashed) and simulated (line) FWHM relative bandwidth of the on-axis spectra.

References:

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Two years of User Operation at European XFEL

EuXFEL

2019 was the second year of user operation at European XFEL, and since 6 May all instruments are operational. More than 1200 users from all over the world visited the facility, and more than 90 experiments were carried out over more than 5000 hours of beamtime. Research topics are diverse and address issues in health, demographic change, clean and efficient energy, climate and environmental research as well as enabling technologies. In this newsletter we would like to share some recent examples.

In one research highlight, an international team led by Stewart McWilliams from the University of Edinburgh used the intense laser flashes to heat and analyse samples in so-called diamond anvil cells at the European XFEL's HED instrument for the first time. In diamond anvil cells (DAC), two small and ultra-hard diamond anvils compress tiny samples, generating pressures similar to those prevailing in the interior of the earth. For their experiment the researchers put a new interaction chamber at HED into operation. The vacuum chamber features a revolving plate holding up to 6 DACs for quick exchange, two large-area detectors for the diffraction patterns as well as an optical system for imaging the samples and non-contact temperature measurement. The setup was developed for the European XFEL by DESY as part of the consortium Helmholtz International Beamline for Extreme Fields (HIBEF), in which a number of institutes under the leadership of the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) have joined forces.

In another paper recently published in Nature Methods, scientists led by Marius Schmidt from the University of Wisconsin-Milwaukee showed how to effectively use the high X-ray pulse repetition rate of the European XFEL to produce detailed molecular movies. They show how measurements can be taken close enough together to maximize the amount of data collected, while making sure that the sample being studied is not hit by anything but the intended laser pulse. For their experiments, the scientists studied a light-sensitive protein known as photoactive yellow protein (PYP), which is often used by scientists as a model system to evaluate new experimental setups. Results matched those obtained from data collected during previous experiments at other facilities, proving their setup was collecting valid data. They were also able to access a previously uncharted time range revealing novel details about parts of the biological reaction.

And in a paper published in *Nature Communications* led by Petra Fromme from Arizona State University (ASU), an international group of scientists showed that the fast X-ray pulse rate produced by the European XFEL can be used to study the structure of membrane proteins such as those involved in photosynthesis. The data presented in the study shows the structure of photosystem I in the so-called dark state, before being activated by light to start the process of converting light to energy via photosynthesis. It is the first membrane protein to be successfully studied at the facility and shows the first proof of concept of megahertz serial crystallography with one of the largest and most complex membrane proteins in photosynthesis. The work paves the way towards time-resolved studies at the EuXFEL, such as molecular movies of the light-driven path of the electrons in photosynthesis or visualizing how cancer drugs attack malfunctioning proteins.

To be able to host the increasing number of users and visiting scientists on the campus, European XFEL started construction of a guesthouse in November. The building, which is scheduled to open its doors in 2021, will have 58 beds in 55 rooms and be equipped with modern and functional facilities.

Bernd Ebeling

Steering Committee Meeting at PSI

The Paul Scherrer Institut (Villigen - PSI) hosted on 20 and 21 November 2019 the meeting of the Steering Committee (SC) of FELs of Europe (FoE). Representatives of 9 FoE partners attended the SC meeting, which was organized after the 2019 LEAPS Plenary Meeting, event hosted by PSI as well.

After the approval of some changes in the organization 2020-2022 and of the provisional budget for 2020, the SC examined the status of the activities of the FoE expert working groups; in this context it was decided to hold the 2nd Forum for Advanced FEL techniques in connection to the Science@FEL conference at DESY in September 2020. In other fields, like photon pulse length measurement and instrumentation, the decision was to explore similar initiatives connected to the PhotonDiag workshop and to explore possible interactions and synergies with the LEAPS working groups.

The progress in the preparation of the two FoE events in 2020, namely the Science@FEL conference at DESY/XFEL from 14 to 17 September and the PhotonDiag workshop at PSI from 26 to 29 October, was then reported. Preparation activities are progressing smoothly and quite soon there will be the official websites available and registration will start. At the meeting the selection of possible candidates as hosts for the 2022 events has started as well.

It was also agreed that FoE will take a stimulating role in organizing a meeting between all soft X-rays FELs and infrared FELs to discuss specific topics of common interest, for both the accelerator part and the photon part, as it is happening already for the hard X-rays facilities (the so called "5 ways meeting"). This idea will be further developed.

. Michele Svandrlik

PhotonDiag 2020

The 5th FELs OF EUROPE workshop on FEL Photon Diagnostics, Instrumentation and Beamline Design, PhotonDiag, will take place at the Paul Scherrer Institut (PSI) from **26 to 28 October 2020**.

There will be also Satellite Meetings on 29 October 2020.

Due to Covid-19 constrains, the conference has switched to a Telco format that will mix pre-recorded talks with poster- and workshop sessions that are attended virtually by live participants. The abstract submission deadline has adapted and extended accordingly. For actual information about the conference status and registration link to the conference homepage https://indico.psi.ch/event/7531/.

The PhotoDiag 2020 conference deals with new developments and advances in the field of photon diagnostics, ranging from new devices for online measurements, to data processing, new experimental challenges and future developments for next generation X-ray light sources. A set of satellite meetings enhances important topics such as soft X- ray photon diagnostics, single-shot pulse energy measurements, wavefront characterization and correction, pulse length measurements, fast diagnostic data acquisition and others. A list of invited speakers and summary sessions perfect the conference schedule.

The Paul Scherrer Institute PSI is the largest research institute for natural and engineering sciences in Switzerland, conducting cutting-edge research in three main fields: matter and materials, energy and the environment and human health. PSI develops, builds and operates complex large research facilities. PSI is part of the ETH Domain and is located in the Canton of Aargau, in the municipal areas of Villigen and Würenlingen on both sides of the River Aare.

Gregor Knopp

Science@FELs 2020

The International Science@FELs Conference will take place from 14-16 September, 2020 organised by DESY and the European XFEL. Due to the ongoing unclear situation with the COVID-19 pandemic we took the decision to hold the Science@FELs 2020 in Hamburg with an online conference during the same time period. Science@FELs is organised as a regular biannual activity of FELs OF EUROPE, the collaboration of European FEL and SPS Facilities. It will focus on scientific highlights achieved during the last years at FELs and laser facilities world-wide in collaboration also with LaserLab Europe.

The online meeting will incorporate a series of exciting invited talks combined with tutorials for PhD students and young postdocs and a virtual tour of the European XFEL and FLASH. We also plan to host an online poster session to facilitate discussion of new results in the field and invite you to submit abstracts. Further details can be found at the conference website https://indico.desy.de/indico/event/24279/overview No fees occur for this online format.

At the Science@FELs conference, the prize in 'FEL Science and Applications' is awarded in recognition of recent work for scientific excellence in the area of free electron laser science and applications in its broadest sense by a young scientist. The work for which the individual is nominated must be such that a significant component of it was performed during the period 3 years prior to the award. The award is accompanied by a certificate, and a monetary sum of 1000 euros.

As a satellite meeting, a **"Forum on Advanced FEL Techniques"** will take place from **16-17 September** in Hamburg aiming at bringing together FEL experts and users, again in an online format. The goal of the forum is to bring together FEL experts and users. The forum will feature review talks and highlights from both FEL and beamline scientists, which will be followed by extensive discussions in round tables. We plan to have sessions covering coherence, photon pulse manipulation, high pulse energy, polarization control, ultrashort pulses and multiple colours.

Elke Ploenjes

FUSEE: FUture of SEEded Free-Electron-Lasers workshop in Trieste - 2019, 10-11 December

The workshop FUSEE was organised by Elettra Sincrotrone Trieste at the Adriatico Guesthouse (https://www.elettra.trieste.it/Conferences/2019/FUSEE/), and gathered together scientists from several FEL facilities worldwide to debate about the perspectives and challenges in the design of the ultimate seeded FEL source. The large participation, more than 100 scientists from 13 countries around the world, testified the success of the event and the interest in the discussed topics.

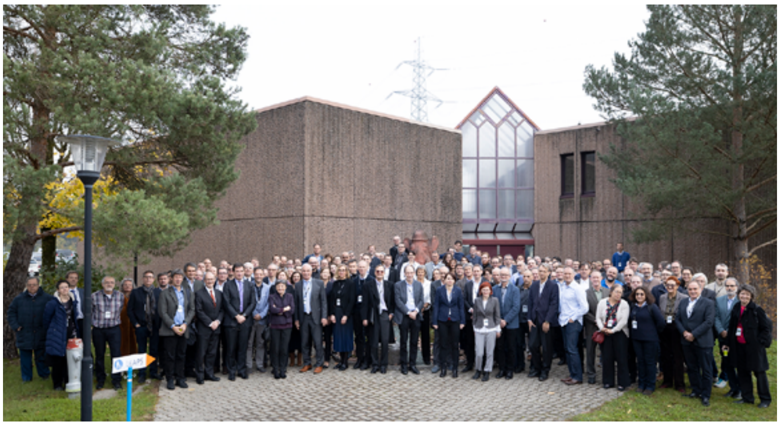
The past few years have witnessed the development of seeded free-electron lasers (FELs), extending the typical optical laser based spectroscopy techniques towards the XUV spectral region. The future plans about the "seeding" techniques and their implementation at the different FEL facilities, both at soft-x ray and hard-x rays, were presented. The discussion comprehended several important aspects, such as the external seeding vs. self-seeding performances, the general question about the photon energy threshold where self-seeding becomes the most reasonable choice with present technologies. Discuss and identify the technological limits in the design of a seeded FEL and the developments that will further extend this photon energy range; identify and compare the most promising schemes aimed at reducing the emission wavelength for external seeded FELs, while preserving the advantages offered by the presence of the seed. Last but not least, identify new issues and propose experiments to solve these issues, and establish collaborations to carry on dedicated experiments.

As to the photon energy extent, at several institutions externally seeded FELs are considered an option up to a photon energy of 1 keV, a range that would include the K-edges of nitrogen and oxygen, and the L-edges of several important transition metals. However, a seeded FEL should be considered as complementary to the existing SASE sources, which may deliver higher peak power and pulse energy, even if with larger shot-to-shot fluctuations and poorer longitudinal coherence.

The discussion during the workshop was enriched and stimulated by the presentations and the contributions of experts in photochemistry, ultrafast coherent soft x-ray imaging, coherent diffraction imaging, x-ray scattering and on the perspectives opened by seeded FELs in chemistry and biology. Users pointed out the key characteristics of FEL pulses needed to fulfil their experimental expectations. Conditions exist where a deterministic source gives advantages with respect to SASE in terms of statistics which can be as high as 10^4. The outcome of the workshop underlines the importance of pushing the present technological limits for seeded FELs feeding with this special light more and more new experiments.

As an opportunity of discussion on the technical aspects between the machine physics and the user community, this workshop constitutes a follow up of the 2018 Forum on Advanced FEL Techniques, the satellite event to the biannual Science@FEL conference. The next edition of the Forum is foreseen in Hamburg, September 16-17, 2020.

Luca Giannessi and Claudio Masciovecchio



More than 180 people gathered for the second LEAPS Plenary meeting at Paul Scherrer Institut.

LEAPS benefits all of Europe

The second LEAPS Plenary meeting was held at Paul Scherrer Institut in Villigen, Switzerland on 18–19 November. More than 180 participants from around Europe met up to discuss how the LEAPS Programme should be developed to best meet the needs and expectations from scientists using the facilities, from the funders and society at large.

The first day of the meeting offered presentations on LEAPS status, ExPaNDs and PaNOSC, and updates on LENS and SESAME as well as meetings within the workgroups and strategy groups of LEAPS.

The second day of the Plenary contained presentations, panel discussions and meetings within the workgroups and strategy groups. Adam Tyson, Head of Unit, Research & Industrial Infrastructures, European Commission gave a very well received talk and pointed out that "the new vision and priorities set out by President-elect Ursula von der Leyen are all issues where research and innovation have a strong role to play. It is a fantastic opportunity but also a very big responsibility for all stakeholders in the field." The input given during these two days will lead to a comprehensive LEAPS Programme well suited to make the most effective contribution possible to the Horizon Europe missions and grand challenges throughout the next decade and beyond.

Tutti Johansson Falk

CURRENT AND UPCOMING CALLS FOR PROPOSALS

www.fels-of-europe.eu/user_area/call_for_proposals

For experiments at FELBE
Deadline: 15 October 2020

For experiments at FELIX
Deadline: 15 November 2020

For experiments at FERMI FEL-1 and FEL-2 at Elettra
Deadline: mid November

For experiments at FLASH
Deadline: Due to planned upgrade work, there will be no further call in 2020

UPCOMING EVENTS

Science @ FELs conference
14-16 September 2020 (online)

PhotonDiag 2020 conference
26-29 October 2020 (online)

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FELs OF EUROPE is an initiative of the ESFRI projects EuroFEL and European XFEL. It is a collaboration of all free electron laser (FEL) facilities in Europe, with the goal to meet the technological and scientific challenges of these novel and rapidly developing technologies and to provide a worldwide unique, pan-European research infrastructure that enables exploiting the full scientific potential of these unique accelerator based short-pulse light sources. More info at: www.fels-of-europe.eu