
ANNUAL REPORT
2020
European
XFEL
Developments, Results, Impressions
SLC2445ws-B

Contents

Foreword 2020

The year 2020 will go down in history as a very special year, also at European XFEL: It started out very well for us, with a Users' Meeting in January that again featured a record number of participants and excellent presentations of experiments done at the facility. It was really great to see, for the first time, such a broad spectrum of research from all of our scientific instruments. The prospects for new scientific discoveries in 2020 were great and, in February, the proposal review panels assessed an exciting set of proposals for experiments.

User experiments started as planned in March, but shortly afterwards we were overrun by the pandemic in the second week of the month, and countries all over the world went into lockdown. We will never forget when some our users had to leave the facility in the middle of the night to catch the last plane home to the USA, while others continued their measurements until the very end of the beam delivery. This was the morning of Monday, 16 March. In the management board, we had to take decisions that we had never imagined would be necessary. An extraordinary staff meeting, the last in-person gathering for more than a year, was held on Friday, 13 March, where staff members were informed that the company would go into a reduced mode of operation in which nearly all staff had to work from home. The shift to home office functioned exceptionally well, due to fantastic efforts by our IT & Data Management (ITDM) and Legal groups, with the help of many others. From one day to another, everything was done online: seminars, routine staff meetings, interviews, Council and committee meetings, and social events. Extremely quickly, we all became Zoom experts, learning by doing how to mute and unmute our microphones, share our screens, and so on. We also quickly introduced a new internal communication platform, on which all staff members could share news and achievements from their groups as well as social activities.

Nearly the entire user programme—with many exciting experiments we had been looking forward to—had to be shifted to the second half of 2020 or even to 2021. Together with the DESY Directorate, we decided to put the accelerator into a safe shutdown mode to prevent mechanical damage in case of an uncontrolled warmup. The period from mid-March to early May, before the restart of the accelerator, was nevertheless very productive. Many important tasks that had been postponed, due to the time pressure of operation, were performed, including data analysis and writing of scientific and technical papers as well as documentation, programming, risk assessment, and so on.

Fortunately, we were able to restart the facility relatively quickly and could start user operation in the fall. However, nearly all user experiments had to be postponed and rescheduled, and, due to travel restrictions, most users were not able to come on site. In fact, during the fall, we registered only 16 users on site, mostly from the local area. Also, important commissioning work had to be postponed, including the split-and-delay line at the MID instrument, commissioning of the DIPOLE laser at the HED instrument, and testing the new beam shutter systems that would allow more X-ray pulses in the experiment hall.

However, we also quickly realized our role in fighting the pandemic. Our XBI biology laboratories for instance could immediately help in this important task, and our lab experts worked closely with scientists from the Hamburg area in the fight against the pandemic by identifying potential drug candidates using the excellent tools for mass spectrometry available in our labs.

It also became rapidly clear that the pandemic could only be conquered by developing vaccines, and that such a development had to be based on science and technology, where our expertise and capabilities in bio-crystallography could be helpful. Hence, we issued a rapid call for COVID-19–related experiment proposals. The deadline for the call was in June, and, with Scientific Advisory Committee (SAC) support and the help of the Peer Review Panel (PRP), the proposals were quickly reviewed, so first beamtime could be allocated for November, with the remaining experiments to be performed in spring 2021.

1: Robert Feidenhans'l, 2: Nicole Elleuche,
3: Serguei Molodtsov, 4: Sakura Pascarelli, 5: Thomas Tschentscher

By August, most of us thought that the worst was over and that we were on the way back to normality. Under the circumstances, the fall went well, and a range of exciting experiments was performed at all instruments, the highlights of which you can read about in this report.

As the winter of 2020–2021 showed, the world would not get out of the grips of the pandemic as easily as we had hoped. With only a limited number of staff members on site, social activities and scientific interactions are at least partially missing. We miss the daily small talk with staff members in which we get the newest and most interesting information about progress within the company. We are confident, that the pandemic situation will improve by fall 2021 and that more life will return to campus soon.

Robert Feidenhans'l

Nicole Elleuche

Managing Directors

Serguei Molodtsov

Sakura Pascarelli

Thomas Tschentscher

Scientific Directors

Maria Faury – Chairperson of the European XFEL Council

Council Chair Foreword

Life is definitely not a walk in the park, and the COVID-19 pandemic has brought us its share of inconveniences. But, as Albert Einstein said, “in the middle of difficulty lies opportunity”, and I believe that European XFEL has grown stronger through this crisis.

It has been an unprecedented year, starting with the lockdown in March, the shutdown of the accelerator to safe mode, and the implementation of massive home-working. Unprecedented decisions had to be made, and the Council commended the European XFEL management for their responsive and responsible approach. Despite all the burdens, the management and the staff have maintained the performance and progress of the company in an impressive way with a successful, if restricted, user programme during the fall with most users online.

The Council has again been very active this year, taking important decisions for the future, giving its green light for the HiBEF user consortium Agreement and for the building of a third instrument at the SASE3 beamline. Many delegates are actively involved in a working group dealing with potential actions to mitigate the impact of the transition from share- to usage-based cost repartition. Following their recommendation, the Council decided to postpone the transition from 2023 to 2024 in order to get more robust statistics. In November, the Council expressed its strong support for the development of a strategy for the next decade and beyond.

In 2021, I am happy to welcome Sabine Carl from the German Federal Ministry of Education and Research (BMBF) as the new Chair of the Administrative and Finance Committee (AFC). And I would like to thank Xavier Reymond for the tremendous work he has done in this position with professionalism and a constructive spirit.

There are still many uncertainties ahead of us, and the start of 2021 is still overshadowed by the pandemic and lockdown restrictions, impacting the restart of the facility as well as the user programme after the winter shutdown. However, European XFEL is prepared for further challenges, so this shall not prevent us from welcoming the new year with prudent optimism and inspiration.

Again, I would like to thank the management, the staff, the governance bodies and the scientific community for their deep involvement and strong commitment to the success of European XFEL—today and in the future. Thank you for keeping us enlightened!

Maria Faury

HIGHLIGHTS

The REMI endstation at SQS being prepared for experiments

Tracking the ultrafast dynamics of photoinduced spin state switching in metallogrid complexes

Maria A. Naumova, Deutsches Elektronen-Synchrotron, Germany
Sophie E. Canton, ELI Attosecond Light Pulse Source, Hungary

Polynuclear complexes incorporating several transition metal ions are intensively investigated for their prospective photoconversion applications. Their rational design crucially depends on charting detailed maps of the energy and charge flows following photoabsorption. In contrast to mononuclear complexes, which involve only one metal ion, the photoinduced dynamics in polynuclear complexes remain scarcely studied to date due to the intricacies associated with the numerous competing channels. In particular, the intrinsic rates of spin state transition cannot be accessed with transient absorption spectroscopies in the ultraviolet, visible, and infrared range. In an experiment at the FXE instrument of the European XFEL, we employed femtosecond X-ray emission spectroscopy to directly track the ultrafast dynamics of photoinduced spin state switching within two metallogrid complexes containing three and four iron ions, respectively. In combination with complementary spectroscopic observations, it was possible to unequivocally reveal the definite impact of nuclearity—that is, the number of metal ions—on the photoinduced dynamics. More generally, our study paves the way to the systematic development of novel polynuclear complexes optimized for photoconversion with energy-rich excited states.

Transition metal complexes (TMCs) are primary building blocks ubiquitous in chemistry and materials science. Linking several TMCs into organized assemblies is an efficient synthesis strategy frequently adopted to augment the performance of photoconversion applications. For example, compact arrays of TMCs tend to exhibit wider spectral coverage with higher extinction coefficient than single chromophores.

Following efficient photoabsorption, the Franck–Condon excited state decays to a thermalized metastable state through a complex interplay between intersystem crossing, charge transfer, structural rearrangements, and energy dissipation, which can all be influenced by the nuclearity of the assembly. Identifying the numerous deactivation pathways is a prerequisite for maximizing the yield of the metastable state and extending its lifetime into the regime of diffusive processes in order to ensure its subsequent reactivity. To gain this understanding, the coupled dynamics of the spin, electronic, and nuclear degrees of freedom need to be exhaustively mapped on an ultrafast time scale. Owing to its intrinsic elemental and spin sensitivity, femtosecond X-ray emission spectroscopy (XES) is uniquely suited for monitoring the dynamical changes in spin multiplicity across the full manifold of excited states.

Building on the pioneering work on mononuclear iron (Fe) complexes performed over the last decade at X-ray FEL sources worldwide, we applied this technique to track for the first time the ultrafast dynamics of photoinduced spin state switching in two homometallic grid-like complexes containing three and four Fe(II) centres, respectively [1, 2]. The structures of the complexes, denoted Fe3 and Fe4, are displayed in Figure 1a. In the solution phase, Fe3 primarily contains two Fe centres in the low-spin (LS) state (blue dots) and one Fe centre in the high-spin (HS) state (red dots), denoted 2LS-1HS. Fe4 consists of 39% in the 2LS-2HS state and 61% in the 1LS-3HS state (Figure 1b).

The XES measurements of the $K\alpha_{1,2}$ and $K\beta$ emission lines were performed at the FXE instrument of the European XFEL [3]. Solutions of Fe3 and Fe4 acetonitrile were delivered as a thin liquid sheet into the interaction region where the optical laser pump pulses (400 nm and 515 nm) and the X-ray probe pulses (9.3 keV) overlapped in both space and time. The signals were collected as a function of the variable pump–probe delay Δt using an energy-dispersive von Hamos spectrometer and a 2D CCD Greateyes detector. The transient difference XES (ΔXES) spectra were obtained by subtracting the "laser off" XES signals from the "laser on" XES signals after background removal and normalization. Figure 1c shows the ΔXES spectra of the $K\alpha_{1,2}$ and $K\beta$ lines for Fe3 at Δt = 1 ps, along with the respective differences of reference lineshapes. The profile characteristic for the formation of an HS state appears quasi-instantaneously, considering the time resolution that was achievable in the experiment (~330 fs) [3]. The kinetics of the photoinduced process can be captured by following the temporal evolution of the integrated areas of the ΔXES profiles. Fitting with a Gaussian-broadened step function yields the time constant of the spin-switching process (Figure 1d).

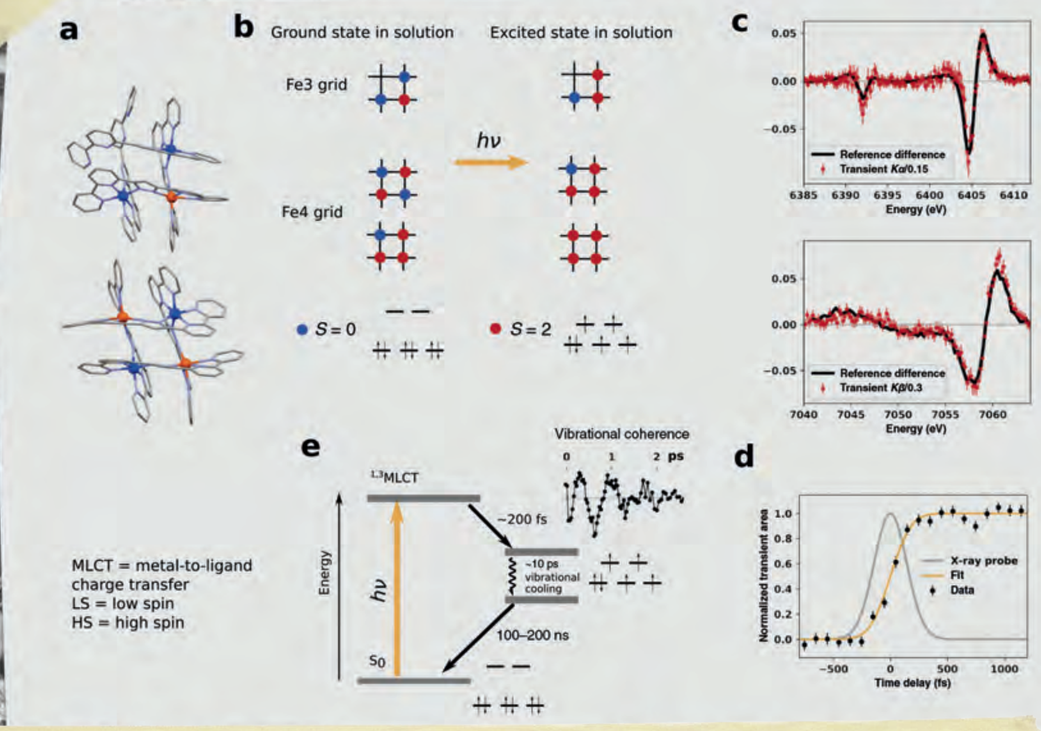

Figure 1: XES measurements of Fe metallogrid complexes at the FXE instrument. (a) Molecular structures of Fe3 and Fe4 from density-functional theory (DFT). (b) Location of the LS (blue) and HS (red) Fe atoms in the ground and excited states of Fe3 and Fe4 in acetonitrile. (c) Red dots: transient $K\alpha_{1,2}$ signals at Δt = 1 ps for Fe3 after 515 nm excitation (top); transient $K\beta$ spectrum at Δt = 1 ps after 400 nm excitation (bottom). Black lines: reference traces constructed by subtracting the static line shapes for LS and HS mononuclear complexes. The transient spectra are scaled to match the references. (d) For Fe3: area under the transient $K\alpha_1$ emission line (6400.2–6409.4 eV) as a function of the time delay between the laser and X-ray pulses; fit with a Gaussian-broadened step function. (e) Photocycle for Fe3 and Fe4. The inset shows the vibrational coherence observed in the optical spectra.

Combining these observations with the results from complementary femtosecond absorption measurements in the ultraviolet, visible, and infrared ranges allows us to propose the reversible photocycle displayed in Figure 1e. Photoabsorption by an Fe centre in the LS state yields a vibrationally hot HS state that exhibits coherent behaviour over the first 1–2 ps. Vibrational cooling to the thermalized HS state takes place within tens of picoseconds. The lifetimes of the metastable states are drastically prolonged compared to closely related mononuclear complexes (123 ns for Fe3, 210 ns for Fe4).

These experimental findings demonstrate that the nuclearity has a profound impact on the photoinduced dynamics. They also reveal the unique potential of Fe3, Fe4, and other Fe metallogrids as advanced photoreactants [4, 5]. Based on the present work, future studies will focus on hetero-metallogrids where the spin state transition is coupled to intramolecular electron transfer in order to realize synergistic energy, charge, and spin manipulation.

Authors

M.A. Naumova, A. Kalinko, J.W.L. Wong, M. Abdellah, H. Geng, S.A. Gutierrez, J. Meng, M. Liang, P.-A. Mante, W. Lin, P. Zalden, A. Galler, F. Lima, K. Kubicek, M. Biednov, S. Checchia, E. Domenichini, A. Britz, V. Kabanova, M. Wulff, J. Zimara, D. Schwarzer, S. Demeshko, V. Murzin, D. Gosztola, M. Jarenmark, J. Zhang, M. Bauer, L.M. Lawson Daku, W. Gawelda, D. Khakhulin, C. Bressler, F. Meyer, K. Zheng, S.E. Canton

References

[1] M. Steinert et al.: "A trinuclear defect-grid iron(II) spin crossover complex with a large hysteresis loop that is readily silenced by solvent vapor", Angew. Chem. Int. Ed. **53**, 6135–6139 (2014), doi:10.1002/anie.201403068
[2] B. Schneider et al.: "A double-switching multistable Fe4 grid complex with stepwise spin-crossover and redox transitions," Angew. Chem. Int. Ed. **49**, 9274–9277 (2010), doi:10.1002/anie.201001536
[3] D. Khakhulin et al.: "Ultrafast X-ray photochemistry at European XFEL: Capabilities of the Femtosecond X-ray Experiments (FXE) instrument", Appl. Sci. **10**(3), 995 (2020), doi:10.3390/app10030995
[4] M. A. Naumova et al.: "Revealing hot and long-lived metastable spin states in the photoinduced switching of solvated metallogrid complexes with femtosecond optical and X-ray spectroscopies", J. Phys. Chem. Lett. **11**, 2133–2141 (2020), doi:10.1021/acs.jpclett.9b03883
[5] M. A. Naumova et al.: "Exploring the light-induced dynamics in solvated metallogrid complexes with femtosecond pulses across the electromagnetic spectrum", J. Chem. Phys. 152, 214301 (2020), doi:10.1063/1.5138641

Probing nanoscale dynamics with MHz repetition rates

Felix Lehmkühler,
Deutsches Elektronen-Synchrotron DESY, Germany

Dynamics and kinetics in soft-matter physics, biology, and nanoscience frequently occur on (sub-) microsecond time scales, which are difficult to probe experimentally. The European XFEL enables such experiments down to atomic length scales for the first time, thanks to its MHz repetition rate. We used microsecond X-ray photon correlation spectroscopy (XPCS) at the SPB/SFX instrument to observe the dynamics of nanoparticles dispersed in water. In the experiment, series of speckle patterns were measured with sub-microsecond time resolution. We found exceptional stability over the pulse train, suggesting very weak—if any—shot-to-shot fluctuations of beam size, pointing, and coherence. By fine-tuning the fluence of the European XFEL pulses, we were able to observe different degrees of beam-induced heating. At fluences above 50 mJ/mm², superheated-water states above 170°C were reached, which persisted at least for 100 µs.

In the last decade, hard X-ray FELs have opened up new research directions. These facilities hold special promise for the investigation of equilibrium and non-equilibrium processes with XPCS [1]. Whereas at storage ring light sources, XPCS typically enables studies of dynamics between milliseconds and hours in real time, the time scale accessible at FELs is defined by the pulse repetition rate. The unique pulse scheme at the European XFEL allows studies of (sub-)microsecond dynamics by exploiting the MHz repetition rate within the pulse trains in such XPCS experiments. These temporal regimes correspond to the natural time scale of diffusion processes of nanoparticles and biological macromolecules in their native aqueous environment. We explored this time scale in the first experiment in which the MHz repetition rate of the European XFEL was a crucial requirement. The study revealed the dynamics of colloidal nanoparticles as a model system for nanoscale materials.

The scheme of the experiment carried out at the SPB/SFX instrument [2] is shown in Figure 1. Pulse trains of 120 X-ray pulses at a photon energy of 9.3 keV, with a size of 3.6 µm x 4.4 µm and a repetition rate of 1.128 MHz, corresponding to a time interval of 886 ns between the pulses, hit a fresh spot of the colloidal sample every 100 ms. The coherent diffraction patterns—called speckle patterns—were measured using the SPB/SFX AGIPD detector.

As a coherent X-ray scattering technique, XPCS relies on the coherence properties of the X-ray pulses. The sample dynamics are obtained from intensity–intensity correlation functions from successive X-ray pulses, which are modelled, among others, using the Stokes–Einstein relation for diffusion of spherical particles through a liquid. The pointing stability during the pulse train is of utmost importance because these correlations are calculated from different X-ray pulses. Pulse-to-pulse SASE fluctuations have been observed in previous XPCS experiments at other FEL sources [3, 4, 5]. The degree of such fluctuations can be quantified by comparing the speckle contrast from single-pulse speckle patterns with the contrast obtained from the intensity–intensity correlation function from static samples. We found that both values match, which shows that the European XFEL provides unprecedented beam stability within a pulse train.

In our XPCS experiment, we used silica nanoparticles with a radius of 69 nm that were dispersed in water as model samples for nanoscale materials. Different X-ray fluences between 1.3 and 56.8 mJ/mm² per single pulse were applied. Some results from a single pulse train are shown in Figure 2. The measured diffusion coefficients resemble the results from theory when low fluences are used. Increasing the fluence leads to a speeding up of the particle dynamics.

Due to the exceptionally high intensity of the European XFEL pulses, the exposed sample volume heats up instantaneously. Subsequently, its temperature relaxes back. While this scenario has been observed at the LCLS and SACLA X-ray lasers in the USA and Japan, respectively [3, 4, 5], it is not fully valid here because the temperature relaxation time is longer than the pulse repetition rate [1]. Consequently, the next pulse hits a non-equilibrated sample, resulting in a stepwise increase in temperature and thus a speeding up of the sample dynamics.

In order to quantify this process, we performed a pulse-resolved XPCS analysis. For this purpose, diffusion coefficients were extracted after each pulse, giving access to a pulse-resolved effective temperature (Figure 3). At a fluence of 56.8 mJ/mm²—while the sample was still in the liquid phase, as evidenced by the diffusive dynamics of the nanoparticles—the effective temperature crossed the boiling point of water and rose to superheated states at about 445 K at the end of the pulse train. This heating exceeded the heating of pure water (dashed lines). It could be modelled taking into account the explicit time resolution of heat relaxation and convective heat transfer between the nanoparticles and the water (solid lines). However, at short times and large T_{eff}, both models fail, suggesting that the nanoparticles move faster than what is expected from the Stokes–Einstein relation. This motivates further studies on heat transfer at the nanoscale to understand the emergence of non-equilibrium dynamics in liquids and soft matter probed at MHz X-ray FEL sources.

To conclude, our study demonstrated the application of XPCS at the European XFEL. Currently, XPCS is further used in various studies at the MID instrument and will be extended to femtosecond and picosecond time scales using the MID split-and-delay line.

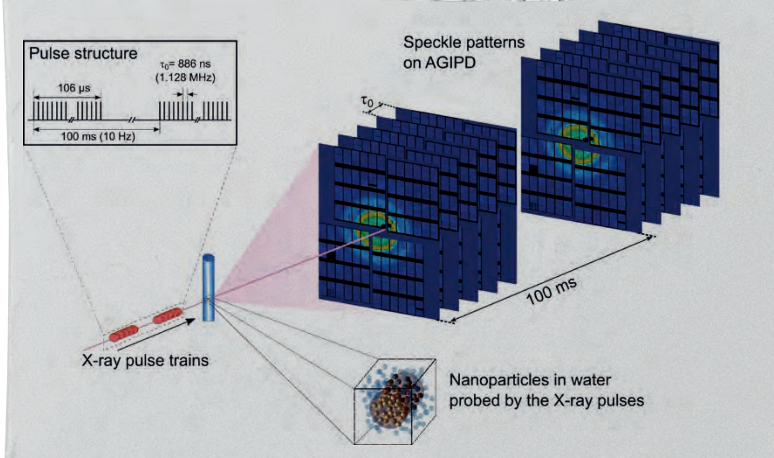

Figure 1: Sketch of the experiment at the SPB/SFX instrument. The X-ray pulse trains scattered off the sample filled in quartz capillaries. The speckle patterns were recorded in small-angle scattering geometry 5.5 m downstream of the sample by the AGIPD detector. The pulse trains contained 120 pulses each and were separated by 0.1 s. Within each pulse train, consecutive pulses were separated by 886 ns (1.128 MHz repetition rate).

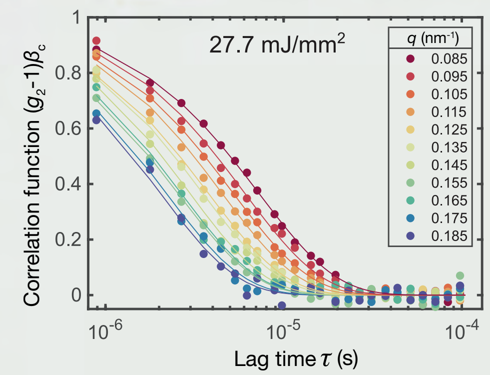

Figure 2: Normalized correlation function g_2 measured in real time from a single train of 120 pulses at a fluence of 27.7 mJ/mm². Solid lines are fits to the data.

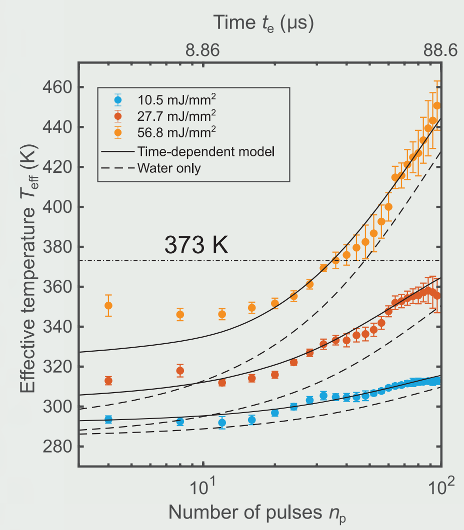

Figure 3: Effective temperature T_{eff} as a function of the pulse number in the pulse train (n_p) for different fluences. The black lines represent the time-dependent heating model, the dashed lines the heating of water as solvent only. The boiling temperature of water is given by the horizontal dashed-dotted line.

Authors

F. Lehmkühler, F. Dallari, A. Jain, M. Sikorski, J. Möller, L. Frenzel, I. Lokteva, G. Mills, M. Walther, H. Sinn, F. Schulz, M. Dartsch, V. Markmann, R. Bean, Y. Kim, P. Vagovic, A. Madsen, A.P. Mancuso, G. Grübel:
"Emergence of anomalous dynamics in soft matter probed at the European XFEL", Proc. Natl. Acad. Sci. USA **117**, 24110–24116 (2020), doi:10.1073/pnas.2003337117

References

[1] G. Grübel, G.B. Stephenson, C. Gutt, H. Sinn, T. Tschentscher: "XPCS at the European X-ray free electron laser facility", Nucl. Instrum. Meth. B **262**, 357–367 (2007), doi:10.1016/j.nimb.2007.05.015
[2] A.P. Mancuso et al.: "The Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography instrument of the European XFEL: initial installation", J. Synchrotron Radiat. **26**, 660–676 (2019), doi:10.1107/S1600577519003308
[3] J. Carnis et al.: "Demonstration of feasibility of X-ray free electron laser studies of dynamics of nanoparticles in entangled polymer melts", Sci. Rep. **4**, 6017 (2014), doi:10.1038/srep06017
[4] F. Lehmkühler et al.: "Sequential single shot X-ray photon correlation spectroscopy at the SACLA free electron laser", Sci. Rep. **5**, 17193 (2015), doi:10.1038/srep17193
[5] F. Lehmkühler et al.: "Dynamics of soft nanoparticle suspensions at hard X-ray FEL sources below the radiation damage threshold", IUCrJ **5**, 801–807 (2018), doi:10.1107/S2052252518013696

Opening new vistas on nanoparticle structure

Kartik Ayyer, Max Planck Institute for the Structure and Dynamics of Matter, Germany

X-ray single-particle imaging (SPI) using X-ray FELs holds great promise as a method to determine the structure of individual biomolecules at physiological temperatures without crystallization. In order to realize its potential, one needs to collect enough high-quality diffraction patterns and develop analytical tools to classify their structural variability. In this work, we report on the collection of 10 million patterns on gold nanoparticle test samples in a single beamtime at the SPB/SFX instrument of the European XFEL, setting a blueprint for a new class of SPI experiments. Since nanoparticle synthesis is inherently heterogeneous, the data must be structurally classified to obtain useful 3D structures. We show that the standard methods used previously work relatively poorly and we develop new algorithms to perform the 3D structural sorting that is crucial to imaging such ensembles. In the process, we produce the highest-resolution structure reconstructions using the SPI technique. The experiment also paves the way towards the high-throughput 3D characterization of nanoparticle ensembles.

Coherent diffractive imaging (CDI) is a technique in which objects, when exposed to coherent light, weakly perturb the light waves, leading to the creation of a diffraction pattern on a detector far from the sample [1]. Just as in a textbook Young's double-slit experiment, where the pattern of fringes can be related to the distance between the slits, the diffraction pattern can be used to computationally derive the structure of the objects in the beam. This is also termed "lensless imaging" since one obtains images of the objects without the need for imaging lenses, which are used in conventional microscopy. X-ray SPI is a CDI technique in which coherent X-ray FEL beams are used to sequentially collect diffraction patterns from nanoscale objects, such as nanoparticles or biomolecules (Figure 1). The X-ray beams from FELs like the European XFEL are bright and short enough that the atoms are effectively frozen during the exposure and the signal is generated before the particles get destroyed by the radiation in a process termed "diffraction-before-destruction" [2]. But a single object can still be exposed only once, so in order to obtain 3D structures, data from a large number of particles in random orientations must be combined computationally. Not only do these orientations have to be determined from the data, but any variations in the structure across the different particles must be decomposed. When combined with the fact that the scattering signal from sub-50 nm objects is quite weak and sensitive to background, the technique has been challenging to realize experimentally.

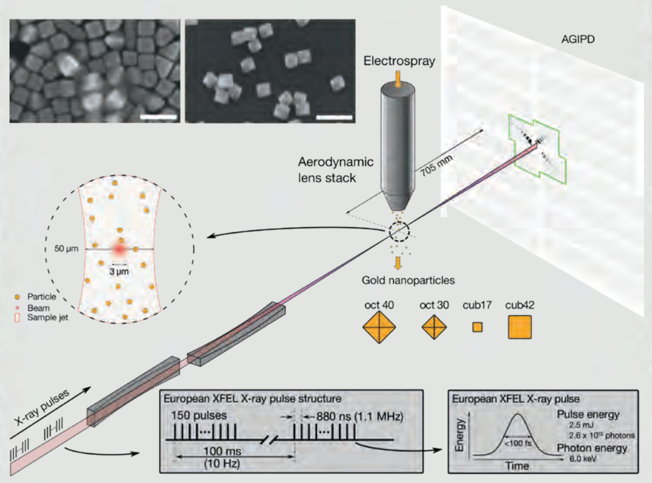

Figure 1: Experiment setup at the SPB/SFX instrument. The European XFEL pulses were focused by a series of Kirkpatrick–Baez mirrors into a 3 x 3 µm² spot and scattered off particles in the aerosol stream to produce diffraction patterns on the AGIPD detector. The lower inset shows the timing structure of the European XFEL pulses at the instrument, while the top inset shows representative scanning electron microscope images of the cub42 and oct30 samples; scale bars are 100 nm. The low-resolution part of the detector used for the structural sorting is highlighted in green.

In 2019, our team of researchers from Germany, Sweden, Singapore, the USA, and Australia came together at the European XFEL to overcome the biggest hurdles in achieving the goal of high-resolution 3D structure determination. These two challenges were the collection of a sufficiently large number of high-quality diffraction patterns and the robust decomposition of structural variability among the particles. The samples chosen were cubic and octahedral gold nanoparticles, which are ideal test samples since they scatter relatively strongly but also have natural structural variability, due to the way they are synthesized. Fully capitalizing on the high repetition rate of the European XFEL, we collected 10 million diffraction patterns over a 60-hour beamtime experiment at the SPB/SFX instrument and reconstructed four structures with sub-3 nm resolution. In the process, we also had to develop algorithms to separate patterns from particles with different structures; otherwise, the reconstruction quality was noticeably worse.

The results of the experiment are exciting for several reasons. First, we were able to demonstrate how the European XFEL is a game changer in terms of being able to collect a truly enormous amount of useful data, which is crucial for the eventual success of the SPI technique. Of course, this also requires a reliable sample delivery system, and the steady developments by various groups have brought us to the point where we were collecting data for up to 10 hours in every 12-hour shift. Using the template set by this work, we are now significantly closer to the long-term goal of visualizing the dynamics of biomolecules with atomic resolution.

The experiment also highlights the power of the serial imaging method for the 3D structure characterization of nanoparticle ensembles. Since each particle is exposed individually, it enables us to identify and image rare events (Figure 2), which would not be possible otherwise, as they would be washed out by the average in an ensemble imaging technique such as powder diffraction or be nearly impossible to find by techniques such as transmission or scanning electron microscopy. And, once you combine this with the fact that the short pulses also enable you to image ultrafast processes, the possibilities are endless.

Authors
K. Ayyer, P.L. Xavier, J. Bielecki, Z. Shen, B.J. Daurer, A.K. Samanta, S. Awel, R. Bean, A. Barty, M. Bergemann, T. Ekeberg, A.D. Estillore, H. Fangohr, K. Giewekemeyer, N.S. Hunter, M. Karnevskiy, R.A. Kirian, H. Kirkwood, Y. Kim, J. Koliyadu, H. Lange, R. Letrun, J. Lübke, T. Michelat, A.J. Morgan, N. Roth, T. Sato, M. Sikorski, F. Schulz, J.C.H. Spence, P. Vagovic, T. Wollweber, L. Worbs, O. Yefanov, Y. Zhuang, F.R.N.C. Maia, D.A. Horke, J. Küpper, N. Duane Loh, A.P. Mancuso, H.N. Chapman: "3D diffractive imaging of nanoparticle ensembles using an X-ray laser", Optica **8**, 15–23 (2021), doi:10.1364/OPTICA.410851

References

[1] H.N. Chapman, K.A. Nugent, "Coherent lensless X-ray imaging", Nature Photon. **4**, 833–839 (2010), doi:10.1038/nphoton.2010.240
[2] H.N. Chapman , A. Barty, M.J. Bogan, S. Boutet, M. Frank, S.P. Hau-Riege et al., "Femtosecond diffractive imaging with a soft-X-ray free-electron laser", Nature Phys. **2**, 839–843 (2006), doi:10.1038/nphys461

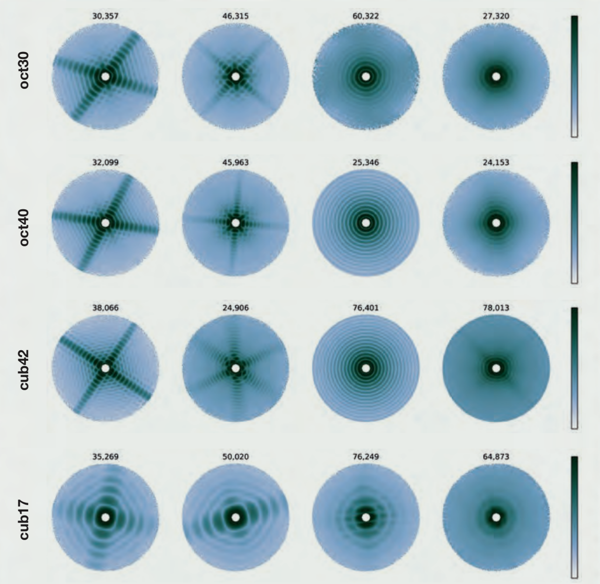

Figure 2: 2D classification. Representative examples of reconstructed 2D models shown on a logarithmic scale, with each row representing a different sample. The numbers indicate how many patterns had that model as the most likely one. The first two columns show models selected for further processing. The third column shows diffraction from rounded/spherical particles, except in the cub17 case, where there were no spherical particles and the model shows diffraction from a dimer instead. The fourth column shows some of the low-contrast models generated by averaging patterns from a diverse set of particles. The resolution at the edge of the circle is 3.3 nm.

Glimpsing the secrets of crystallization

Robert E. Grisenti, GSI Helmholtzzentrum für Schwerionenforschung, Germany
Johannes Möller, European XFEL, Germany

The process of crystallization by which a "super-cooled" liquid—that is, a liquid at some temperature below its melting point—transforms into a solid is one of the most fundamental phase transitions occurring in nature. It substantially determines many physical phenomena, from materials science to atmospheric physics. Microscopic supercooled water droplets at very low temperatures, for example, are naturally present in upper layers of the Earth's atmosphere, such as in aerosol-poor arctic stratiform clouds. Understanding how and at which rates such droplets transform into ice is important because small differences in the ratio of water to ice have a huge impact on the radiative effects of clouds and thus on the development of reliable climate models. Experimentally accessing such details in supercooled liquids is, however, very difficult because of the spontaneous nature and the very short time scale of the crystallization process. To address these challenges, we employ microscopic liquid jets in vacuum in combination with X-ray scattering at the MID instrument of the European XFEL. The unique features of this approach allow us to investigate the early stages of crystallization. Finally, we have the opportunity to shed light on so-far unexplored aspects of the liquid-to-solid phase transition.

Crystallization is generally viewed as a two-step process in which thermal fluctuations in the metastable liquid phase trigger the spontaneous formation of a small, localized seed of the new ordered phase, which subsequently grows to macroscopic dimensions [1]. However, the details of this process, and particularly of the initial nucleus formation commonly known as homogeneous crystal nucleation (HCN), are still very poorly understood. For example, although the classical crystal nucleation theory provides a qualitatively valid description of HCN, theoretical crystal nucleation rates often depart by orders of magnitude from those observed experimentally, and the latter are also found to differ substantially from those predicted by computer simulations. A prominent example that stresses this impasse is supercooled water, for which experimental and numerical crystal nucleation rates can diverge by up to 20 orders of magnitude [2]. A further, highly debated aspect of crystal formation is the possibility, suggested by numerical simulations, of a crystal nucleation process driven by precursor forms with some local symmetry formed within the supercooled liquid, but in fact this scenario is not yet supported by experimental evidence.

Investigations of crystallization in atomic and molecular liquids are extremely challenging because of the inherently stochastic nature of HCN, which greatly hinders access to its details, as no *a priori* knowledge of the exact spatial and temporal coordinates of the spontaneous nucleation event in a macroscopic liquid sample is available. To address this challenge, we combine X-ray pulses from the European XFEL with microscopic liquid jets in vacuum to investigate the early stages of crystallization. The vacuum-exposed jet rapidly cools below melting by surface evaporation until it undergoes a first-order phase transition driven by the onset of HCN [3]. The whole evolution of the crystallization process, from critical seed formation to crystal growth occurring along the jet propagation direction, is effectively mapped onto the time axis through the jet velocity. Information on the structure and size of the rapidly growing crystals is then captured in the single-shot diffraction patterns produced by the ultrashort, intense X-ray pulses, which are focused down to a 300 x 300 nm^2 spot size, scattering off the jet.

In our experiments at the MID instrument [4], we have probed liquid jets of the atomic elements argon and krypton, which are particularly attractive model systems due to their simplicity and because crystallization in these liquids is comparable to that observed in pure metals. A shadow image of a solidified krypton jet generated in the MID sample chamber is presented in Figure 1a. Figure 1b shows the jet explosion during exposure to the focused, non-attenuated X-ray beam. We emphasize that the continuous, self-replenishing nature of the liquid jet allows us, in fact, to take full advantage of the MHz repetition rate of the European XFEL X-ray pulses.

Figure 2a shows averaged scattering patterns clearly revealing the evolution from the liquid phase (bottom panel) to the crystalline phase (top panel), evidencing the characteristic (111) and (200) face-centred cubic (fcc) diffraction rings. Such averaged diffraction patterns resemble those that can be obtained at synchrotron facilities, where long acquisition times make averaging over large sample volumes inevitable. Figure 2b shows difference images obtained from the same data as in Figure 2a by exploiting the pulse-resolved nature of the experiment, allowing for subtraction of the scattering contribution of the liquid fraction. These patterns clearly corroborate the presence of a solidified fraction (bottom panel) that was hidden in Figure 2a and thus demonstrate the feasibility of directly capturing the early stages of crystallization with the intense X-ray pulses of the European XFEL.

At each position along the jet, which, as mentioned earlier, corresponds to a specific temperature of the supercooled liquid, we have recorded over 10^6 single-shot images with the MID AGIPD detector, each of them from a new sample delivered by the jet. The very high repetition rate of the X-ray pulses at the European XFEL has thus allowed us to obtain a valuable data set orders of magnitude larger than in any previous study of HCN, enabling a genuine statistical study of crystallization.

This is important not only to obtain a reliable estimation of the crystal nucleation rate but also to address fundamental aspects related to the structural path during the crystallization process. For example, bulk rare-gas liquids crystallize into the fcc crystal structure, but numerical studies also indicate the formation of a metastable hexagonal close-packed (hcp) solid phase, suggesting that crystallization may proceed with the nucleation and growth of the least stable phase. However, the frequency of the diverse transformation pathways is very difficult to determine, further illustrating the complexity of the phase transition even in such simple liquids.

The data analysis is presently ongoing, but once accurately determined, the resulting crystal nucleation rates and probability distributions for the transformation pathways will offer a unique benchmark for theory and computer simulations in which the particle interaction in the simplest atomic liquids of our study can be reliably described by a Lennard–Jones potential. Ultimately, our results will provide long-awaited experimental input to help guide any future refinements of theories of crystal nucleation and growth in supercooled liquids, thereby advancing our understanding of crystallization.

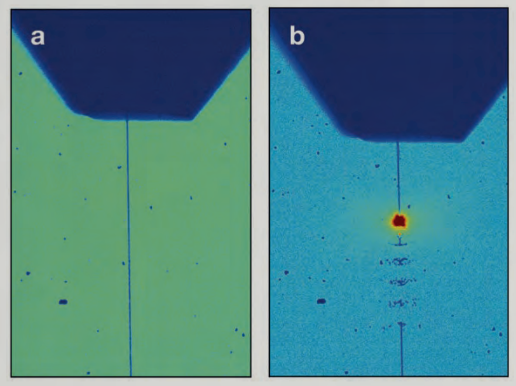

Figure 1: Microscopic images of a krypton jet in the MID sample chamber. (a) Shadow image of a solidified krypton jet ejected at a speed of 100 m/s from a 3.5 µm diameter capillary orifice. (b) Image of the jet after exposure to the focused X-ray beam. X-ray–induced fluorescence can be observed at the interaction spot of the jet and the X-ray beam. The trigger of the laser-based background illumination for the optical camera was set so as to obtain an image of the jet shortly after the fifth X-ray pulse of a train hitting the jet, resulting in four gaps in the jet below the interaction point where argon was blasted away by previous exposures.

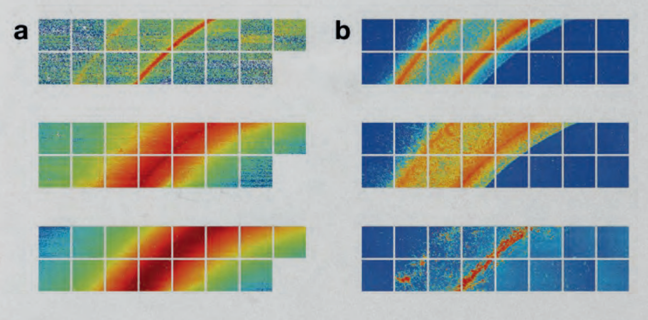

Figure 2: Scattering patterns from a krypton jet. (a) Averaged scattering signal on one of the modules of the MID AGPID detector, with the distance from the capillary orifice increasing from the bottom to the top. (b) Data set obtained from that shown in (a) by displaying the maximum intensities after subtracting the scattering contribution from the liquid.

Authors

J. Möller, U. Bösenberg, F. Dallari, D.E. Galli, L. Gelisio, C. Goy, G. Grübel, A. Kalinin, C. Kim, R. Kurta, D. Lapkin, F. Lehmkühler, A. Madsen, F. Mambretti, A. Schottelius, R. Shayduk, F. Trinter, I. Vartaniants, R.E. Grisenti

References

[1] K.A. Jackson: *Kinetic Processes: Crystal Growth, Diffusion, and Phase Transitions in Materials* (Wiley-VCH Verlag, Weinheim, 2004)
[2] A. Haji-Akbari, P.G. Debenedetti: "Direct calculation of ice homogeneous nucleation rate for a molecular model of water", PNAS **112**, 10582 (2015), doi:10.1073/pnas.1509267112
[3] R.E. Grisenti et al.: "Evaporating laminar microjets for studies of rapidly evolving structural transformations in supercooled liquids", Adv. Phys. X **3**, 1418183 (2018), doi:10.1080/23746149.2017.1418183
[4] A. Madsen et al.: "Materials Imaging and Dynamics (MID) instrument at the European X-ray Free-Electron Laser Facility", J. Synchrotron Radiat. **28** (2) (2021), doi:10.1107/S1600577521001302

Developing an ultrafast thermometer for matter at extremes

Adrien Descamps and Emma E. McBride,
SLAC National Accelerator Laboratory, USA

Warm dense matter is an exotic state on Earth, yet ubiquitous throughout the universe, found in the interiors of stars and giant planets such as Jupiter and Saturn, or even at the centre of the Earth. Typically, such states are generated in the laboratory using high-intensity pulsed lasers to drive either compression waves or rapid heating on femtosecond to nanosecond time scales. These transient states of extreme pressure and temperature are challenging to probe using traditional optical techniques. Hard X-ray FELs, in contrast, provide the ultrabright, ultrashort X-rays pulses necessary to allow these short-lived states to be captured and probed. While inferring density from X-ray diffraction data has become a well-established technique, the measurement of temperature remains a major challenge. Here, we demonstrate a novel first-principles technique at the HED instrument of the European XFEL for measuring temperature using high-resolution inelastic X-ray scattering. This method, combined with the high-repetition-rate lasers available at the HED instrument, will allow new studies to greatly improve our understanding of warm dense matter.

Throughout the universe, matter exists at extremes of pressure and temperature, from the cold vacuum of interstellar space to the hot, dense centres of neutron stars. Particularly intriguing is a state known as warm dense matter, found at the centre of stars and planets as well as in inertial confinement fusion processes. While understanding it is vital for comprehending pathways to fusion energy or creating accurate models of planetary and stellar interiors and their evolution, warm dense matter lies in a pressure–temperature region that is not well described by condensed matter physics or by plasma physics. Therefore, a direct experimental characterization of these states is essential to establish a robust theoretical description.

Extreme states are often created in the laboratory through shock compression using nanosecond laser drivers or through ultrafast heating using femtosecond lasers [1, 2].

The generated states of pressure and density are therefore, by nature, transient, with a large density of free electrons making them challenging to probe using optical techniques. The solution comes with the emergence of hard X-ray FEL sources, such as the European XFEL. These light sources provide extremely bright, time-resolved X-rays with pulse lengths of just few tens of femtoseconds, which can penetrate and probe extreme states. As such, the measurement of the structure and density of compressed matter has become almost routine, providing a wealth of information on the behaviour of these exotic states. However, despite being a vital thermodynamic parameter, temperature remains challenging to measure experimentally.

In such experiments, temperature is often calculated using a hydrodynamic model, which needs to be benchmarked, or is sometimes inferred through the thermal self-emission of a sufficiently hot sample. This latter technique assumes *a priori* knowledge of the material properties, and one accesses only the surface temperature rather than the bulk temperature. In our experiment at the HED instrument, we demonstrated the measurement of bulk temperature in both room temperature and resistively heated single-crystal diamond using ultrafast X-ray pulses. The experiment resolved the diamond phonon modes, whose intensities yield the temperature through the application of the principle of detailed balance. The applicability of this principle was then confirmed using the temperature reading from a thermocouple attached to the sample.

The experiment setup for high-resolution inelastic scattering at the HED instrument is shown in Figure 1 and described in detail in Ref. [3]. While the self-amplified spontaneous emission mode of the European XFEL has a bandwidth of several tens of electronvolts, the X-ray beam was further monochromatized to ~32 meV, sufficient to resolve the characteristic energy transfer for phonon modes, which is typically in the range of tens to hundreds of millielectronvolts. The narrow-band X-ray beam was then scattered from the diamond sample onto

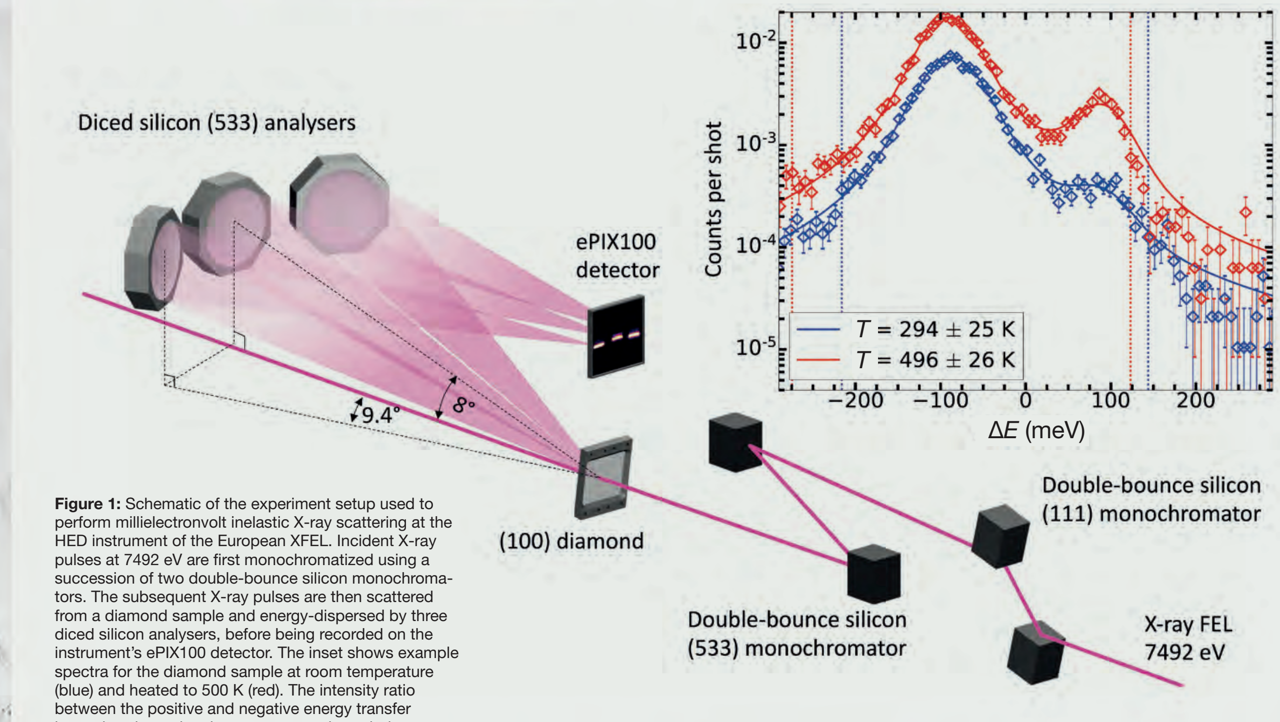

Figure 1: Schematic of the experiment setup used to perform millielectronvolt inelastic X-ray scattering at the HED instrument of the European XFEL. Incident X-ray pulses at 7492 eV are first monochromatized using a succession of two double-bounce silicon monochromators. The subsequent X-ray pulses are then scattered from a diamond sample and energy-dispersed by three diced silicon analysers, before being recorded on the instrument's ePIX100 detector. The inset shows example spectra for the diamond sample at room temperature (blue) and heated to 500 K (red). The intensity ratio between the positive and negative energy transfer is used to determine the temperature through the application of the principle of detailed balance.

three diced and spherically curved single-crystal silicon analysers to obtain the phonon spectrum.

Example phonon spectra from single-crystal diamond, both at room temperature and resistively heated to 500 K, are shown in the inset of Figure 1. We measured only the inelastic Brillouin peaks corresponding to the longitudinal phonon mode along the (100) crystallographic direction, as the sample is a single crystal. The positions of the peaks are related to the sound speed of the material, and the asymmetry of the Stokes and anti-Stokes peaks arises due to Bose–Einstein statistics. The ratio of these peaks allows one to directly obtain the sample temperature. Here, we measured a temperature of 294 ± 25 K for the diamond at room temperature (blue) and 496 ± 26 K when heated to 500 K (red) [4].

Our work demonstrates the feasibility of using inelastic X-ray scattering to measure the bulk temperature of a sample at the HED instrument of the European XFEL. By combining this technique with the high-repetition-rate, high-intensity nanosecond and femtosecond lasers at HED [5], we will soon be able to extend the technique to directly measure the bulk temperature and the material sound speed of transient matter states at extreme pressures and temperatures.

Authors

A. Descamps, B.K. Ofori-Okai, K. Appel, V. Cerantola, A. Comley, J.H. Eggert, L.B. Fletcher, D.O. Gericke, S. Göde, O. Humphries, O. Karnbach, A. Lazicki, R. Loetzsch, D. McGonegle, C.A.J. Palmer, C. Plueckthun, T.R. Preston, R. Redmer, D.G. Senesky, C. Strohm, I. Uschmann, T.G. White, L. Wollenweber, G. Monaco, J.S. Wark, J.B. Hastings, U. Zastrau, G. Gregori, S.H. Glenzer, E.E. McBride

References

[1] D. Kraus et al.: "Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions", Nat. Astron. **1**, 606–611 (2017), doi:10.1038/s41550-017-0219-9
[2] B.I. Cho et al.: "Electronic structure of warm dense copper studied by ultrafast X-ray absorption spectroscopy", Phys. Rev. Lett. **106**, 167601 (2011), doi:10.1103/PhysRevLett.106.167601
[3] L. Wollenweber et al.: "High-resolution inelastic X-ray scattering at the High Energy Density scientific instrument at the European X-Ray Free-Electron Laser", Rev. Sci. Instrum. **92**, 013101 (2021), doi:10.1063/5.0022886
[4] A. Descamps et al.: "An approach for the measurement of the bulk temperature of single crystal diamond using an X-ray free electron laser", Sci. Rep. **10**, 14564 (2020), doi:10.1038/s41598-020-71350-x
[5] P. Mason et al.: "Development of a 100 J, 10 Hz laser for compression experiments at the High Energy Density instrument at the European XFEL", High Power Laser Sci. Eng. **6**, E65 (2018), doi:10.1017/hpl.2018.56

Visualizing spin–lattice coupling in iron–platinum nanoparticles

Hermann Dürr,
Uppsala University, Sweden

Studying the spin dynamics initiated in magnetic materials by a sub-picosecond laser pulse is an emerging and rapidly developing research field in fundamental magnetism, which promises novel applications in information technology. The goal of these studies is to understand and ultimately control the energy and angular-momentum transfer processes occurring in the laser-excited non-equilibrium state. Since the advent of femtosecond optical lasers, research has focused on exploring the electronic and magnetic structure of the excited state. The availability of FEL radiation in the tender and hard X-ray range has recently opened up the possibility to study the coupling of spin excitations to the lattice. In this experiment at the SCS instrument of the European XFEL, we used iron–platinum (FePt) nanoparticles—promising candidates for future high-density magnetic data storage media—to demonstrate the coupling of a ferromagnetic resonance spin precession mode to longitudinal acoustic phonons on a length scale corresponding to the nanoparticle size (~16 nm). We isolated the phonon response using X-ray scattering, which allowed us to probe the ultrafast lattice expansion of the FePt nanoparticles through coherent phonon wave packets, and we detected new modes caused by the non-linear coupling of acoustic phonons to large-angle spin precessions.

The magneto-acoustic coupling of phonon and magnon modes offers novel functionalities for spintronic applications in information technology. Magnon polarons can form by magneto-elastic coupling [1], circularly polarized phonons can form and transport angular momentum [2], and phonons can be used to generate spin currents in metallic contacts [3]. However, many of these phenomena have, so far, been demonstrated only at GHz frequencies and micrometre dimensions. X-ray FELs enable us to explore the potential of moving towards THz frequencies and nanometre dimensions, which are far more attractive for applications.

In this experiment, we have studied the magneto-acoustic coupling of ferromagnetic resonance spin precession modes and acoustic phonons in FePt nanoparticles with an average diameter of around 16 nm. FePt nanoparticles are a promising material for future high-density magnetic data storage media, thanks to their extremely high magnetic anisotropy, which makes them good candidates for pushing back the superparamagnetic limit—a fundamental restriction of the data storage density of hard disk drives due to the minimum size of the particles that can be used.

Figure 1 describes the experiment. A laser pulse induces the propagation of a strain wave through the material from the grain boundaries towards the centre, which results in the expansion of the FePt lattice and grain as a whole (Figure 1a). At the same time, a ~0.2 THz ferromagnetic resonance precession of the FePt magnetization is excited through ultrafast demagnetization with femtosecond optical laser pulses [4].

At the SCS instrument, we detected the laser-induced coherent lattice expansion of the FePt nanoparticles [5] by tender X-ray scattering (Figure 1b), using the instrument's DSSC detector to record the scattering patterns at a photon energy of 2500 eV. X-ray diffraction from the FePt grains in the sample produced a broad scattering ring on the detector with a radius defined by the grain size distribution. We varied the time delay between the laser pump and X-ray FEL probe pulses to explore the temporal behaviour of the system with a resolution down to a few tens of femtoseconds.

The change in intensity of the scattering ring after the arrival of the laser pump pulse depends on the wave vector and shows the dynamics on the sub-picosecond time scale (Figure 1c). Such a wave-vector-dependent scattering yield is a direct probe of coherent acoustic phonon propagation from the perimeter to the interior of the nanoparticles. Surprisingly, in the time domain, we find phonon spectral features of the acoustic phonon mode dispersing with wave vector ***q*** as well as new modes that do not disperse with ***q***. For example, in Figure 1c, the first oscillation corresponding to the acoustic phonon mode appears at a high $q \approx 0.9\ nm^{-1}$ after a time delay of 1 ps and drifts to a lower $q \approx 0.25\ nm^{-1}$ after a time delay of 4 ps. Another feature shows up at 4 ps in a broad q range, being the most distinct at higher $q \approx 0.7–0.9\ nm^{-1}$ and almost merging with the acoustic phonon mode in the middle q range near $0.5–0.6\ nm^{-1}$. Apparently, the non-dispersive features are caused by the coupling between the lattice motion and the ferromagnetic resonance precession of the magnetization. A more detailed analysis (not shown) results in a precession frequency reasonably close to the one observed previously [4].

In conclusion, we have directly visualized, for the first time, the magneto-acoustic coupling in ferromagnetic FePt nanoparticles. This experiment has become possible thanks to the improved performance of X-ray FELs as powerful research tools, which now cover the tender X-ray range. The impact of our research is a better understanding of the basic physical processes in magnetic materials on the nanometre length scale and at THz frequencies, which is highly relevant for state-of-the-art spintronic applications.

Authors

D. Turenne, I. Vaskivkyi, M. Schneider, N. Zhou Hagström, A. Yaroslavtsev, X. Wang, G. Mercurio, L. Le Guyarder, L. Mercadier, J. Brock, D. Mukkattukavil, N. Agarwal, D. Lomidze, M. Turcato, A. Samartsev, M. Teichmann, N. Gerasimova, J. Schlappa, D. Potorochin, B. Van Kuiken, R. Gort, R. Carley, V. Unni, Y. Takashi, S. Molodtsov, A. Scherz, E. Jal, E. Fullerton, S. Bonetti, S. Eisebitt, H.A. Dürr

References

[1] J. Li et al.: "Observation of magnon polarons in a uniaxial antiferromagnetic insulator", Phys. Rev. Lett. **125**, 217201 (2020), doi:10.1103/PhysRevLett.125.217201
[2] J. Holanda et al.: "Detecting the phonon spin in magnon–phonon conversion experiments", Nat. Phys. **14**, 500 (2018), doi:10.1038/s41567-018-0079-y
[3] M. Weiler et al.: "Spin pumping with coherent elastic waves", Phys. Rev. Lett. **108**, 176601 (2012), doi:10.1103/PhysRevLett.108.176601
[4] J. Becker et al.: "Laser induced spin precession in highly anisotropic granular L10 FePt", Appl. Phys. Lett. **104**, 152412 (2014), doi:10.1063/1.4871869
[5] A.H. Reid et al.: "Beyond a phenomenological description of magnetostriction", Nat. Commun. **9**, 388 (2018), doi:10.1038/s41467-017-02730-7

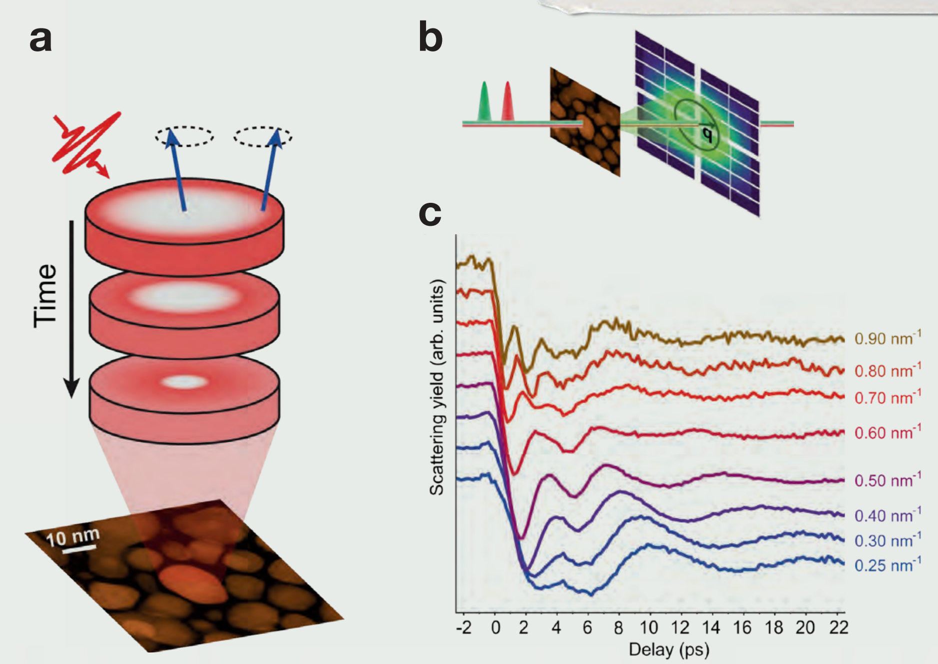

Figure 1: Illustration of the experiment. (a) The process under investigation: Schematic illustration of how femtosecond laser excitation generates spin precession (blue arrows) and lattice expansion propagating via strain waves (red rings) into the interior of the nanoparticle. The transmission electron micrograph at the bottom shows the FePt nanoparticles (brown) suspended in a carbon matrix (black). (b) Schematics of the experiment setup: A femtosecond optical laser pulse ($50\ mJ/cm^2$ fluence) arrives at the sample, followed after a certain time delay by a tender X-ray FEL pulse (2500 eV), which scatters off the nanoparticles and is measured by the DSSC detector of the SCS instrument. (c) Experimental data: Time traces for different ***q*** vectors showing the normalized scattering yield from the nanoparticles. At every ***q***, a number of distinct frequencies are observed, which correspond to the coupled phonon and spin oscillations.

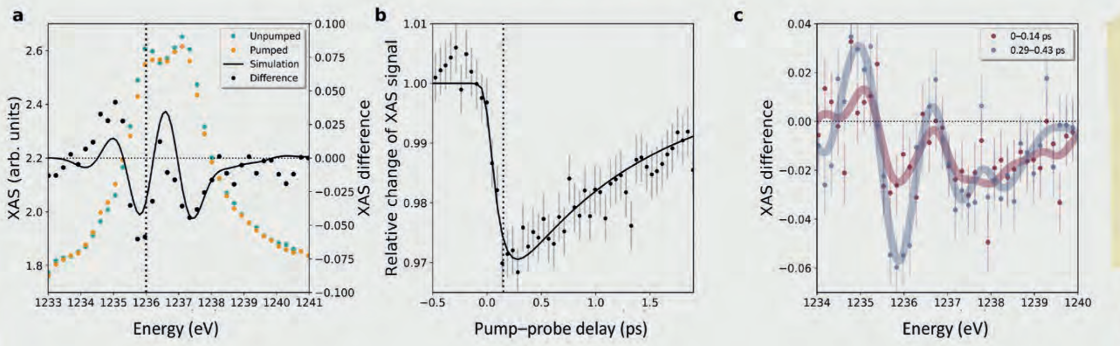

Figure 1: Pump-induced changes of the 4*f* multiplet structure of the rare-earth metal terbium (Tb). (a) 3*d*→4*f* X-ray absorption spectra of Tb for the unpumped sample (cyan dots) and 150 fs after excitation (dashed vertical line in (b)) with 1.55 eV (yellow dots) as well as their difference (black dots). (b) Relative change of the absorption signal measured at 1236 eV (dashed vertical line in (a)). The black line in (b) is a bi-exponential fit with 0.1 ps decay and 1.3 ps recovery constant. (c) Pump effect (XAS difference) for different time intervals showing a change of the 4*f* excitation with time. The thick solid lines in (a) and (c) are guides to the eye.

Observing optically driven 4f orbital transitions in rare-earth metals

Materials with large magnetic anisotropy are required to build high-density magnetic data storage devices. The magnetic properties of these materials differ depending on direction, and the magnetic anisotropy acts like an energy barrier between different magnetization directions. A high anisotropy thus stabilizes stored information against decay but, in turn, also makes it more difficult to write information in the first place. Optimally, one would like to briefly reduce the anisotropy in order to write new information. In a recent experiment at the SCS instrument of the European XFEL, we were able to show, for a high-anisotropy rare-earth metal, that this can indeed be achieved. X-ray absorption spectroscopy (XAS) is sensitive to the orbital state and thus to the magnetic anisotropy of the material. We saw both changing within a few hundred femtoseconds after hitting the material with an ultrashort laser pulse. After a few picoseconds, the original high-anisotropy, high-stability state was restored. Our findings not only demonstrate a potential new approach for magnetic data storage, they also illustrate the importance of soft X-ray spectroscopy with high energy and time resolution, as made possible by the SCS instrument, for understanding fundamental processes in matter.

Nele Thielemann-Kühn,
Freie Universität Berlin,
Germany

The motion of an electron around a nucleus gives rise to electron orbital angular momentum and generates a relativistic magnetic field in which the electron spin aligns in a preferred direction; this mechanism is called spin–orbit coupling (SOC). As the electron orbital angular momentum is in turn coupled to the crystal lattice through the electron motion, it anchors the electron spin magnetic moment to certain crystal orientations. This effect is called magneto-crystalline anisotropy (MCA). How strongly the electron spin magnetic moments are linked to a certain direction is directly connected with the electron orbital magnetic moment. High-density magnetic recording is based on magnetic systems with large MCA. To write bits in these media, the MCA is overcome by briefly heating the spin system above the Curie temperature, above which the material loses its permanent magnetic properties—a technique known as heat-assisted magnetic recording [1].

In a study at the SCS instrument, we found that, instead of pushing the spin system across the MCA barrier, in a 4*f* rare-earth (RE) metal, this barrier itself can be manipulated on femtosecond time scales. Magnetism in RE metals is based on strongly localized 4*f* electrons, carrying the largest magnetic moment among the elements of the periodic table. The 4*f* electrons interact with delocalized 5*d*6*s* valence electrons, which mediate the interatomic 4*f* exchange coupling [2]. SOC is strong in RE metals and leads to high MCA [3]. The European XFEL allows us to address the interplay of 4*f* spin (*S*) and orbital (*L*) degrees of freedom in a direct way. Our approach exploits the fact that any change in *L* and *S* corresponds to an excitation in the 4*f* electronic system. We therefore studied the 3*d*→4*f* X-ray absorption in 4*f* RE metals at the SCS instrument. With that, we could probe the unoccupied 4*f* states with an energy and time resolution sufficiently sensitive to detect changes in the 4*f* electronic structure and connect them to variations of the *S* and *L* degrees of freedom.

We found that, in the 4*f* metal terbium (Tb), whose $4f^8$ electronic configuration causes a large *L* magnetic moment and a huge MCA, the 4*f* electronic state changes on a 100 fs time scale when hit by a laser pulse (Figures 1a and 1b). This change in the 4*f* electronic system resembles the distribution of optically excited 5*d*6*s* electrons [4]. We therefore conclude that the delocalized valence electrons couple to the localized 4*f* electrons. We can simulate the effect on the 4*f* system (black dots and line in Figure 1a) and find that, at early times of up to ~140 fs after optical excitation, the spectral change reveals an occupation of the first excited $4f^8$ state only. Additional excitations occur at later times (Figure 1c), when thermalization of the valence system proceeds and charge carriers form at energies higher than the original pump energy of 1.55 eV above and below the Fermi level E_F (Figure 2b).

The first excited $4f^8$ state, denoted $^7F_5$, lies 0.26 eV above the Tb ground state ($^7F_6$). Inelastic 5*d*↔4*f* scattering with a respective transfer of energy and angular momentum (ΔJ = -1), e.g. through a spin flip in the 5*d* system, allows for occupation of the $^7F_5$ state (Figure 2a). Furthermore, for an internally thermalized 5*d*6*s* system, an electron transfer between the 5*d* and 4*f* system could arise. Hot 5*d* electrons may scatter into the lowest unoccupied Tb $4f^9$ state $^6H_{15/2}$ at 2.8 eV above E_F, or the Tb ground state can be ionized into the Tb $4f^7$ $^8S_{7/2}$ configuration, which requires an energy of 2.3 eV (Figure 2b) [5]. The latter transition corresponds to ΔS = 1/2 and ΔL = -3 and is of special interest for applications, as it reduces the highly anisotropic Tb $4f^8$ configuration to an L = 0 state, which has practically no MCA.

As 4*f* metals play a key role in all optical switching materials, they are of high technological relevance. With our pioneering experiment, which points to the opportunity to control MCA by optical means, this material class becomes even more important for magnetic applications. Besides technological aspects, connecting magnetic dynamics with electronic excitations is an important step towards a more fundamental understanding of magnetic interaction on short time scales and of non-equilibrium magnetic properties in general.

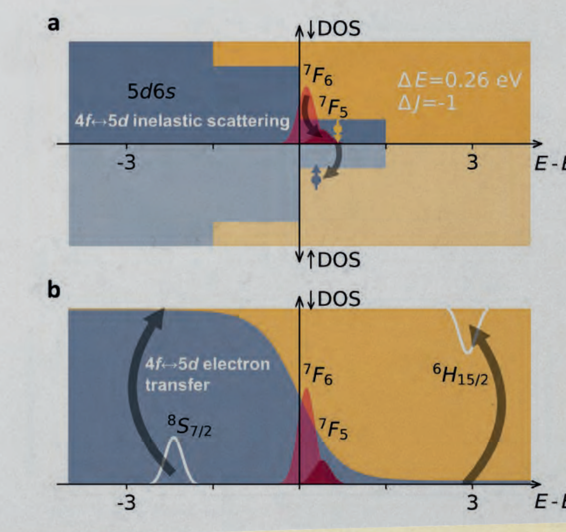

Figure 2: Energy scheme of the involved electronic states. (a) Density of states (DOS) for spin up (↑) and spin down (↓) 5*d*6*s* electrons. The grey (yellow) area denotes the occupied (unoccupied) 5*d*6*s* DOS. The inelastic scattering of localized 4*f* electrons and 5*d* valence electrons photoexcited in the interval of ±1.55 eV around E_F promotes a transition from the Tb $^7F_6$ ground state to the lowest excited $4f^8$ $^7F_5$ multiplet at 0.26 eV. With a spin flip (ΔS = +1) of the 5*d* electron, a momentum transfer of ΔJ = -1 is enabled. (b) The photoexcited 5*d*6*s* electrons form a hot Fermi distribution within 200 fs. By 5*d*↔4*f* electron transfer, the $4f^7$ $^8S_{7/2}$ state 2.3 eV below E_F and the $4f^9$ $^6H_{15/2}$ final state 2.8 eV above E_F can be reached.

Authors
N. Thielemann-Kühn, T. Amrhein, W. Bronsch, S. Jana, N. Pontius, R.Y. Engel, P. S. Miedema, M. Beye, U. Atxitia, B.E. van Kuiken, M. Teichmann, R.E. Carley, L. Mercadier, A. Yaroslavtsev, G. Mercurio, L. Le Guyader, N. Agarwal, A. Scherz, P.M. Oppeneer, M. Weinelt and C. Schüßler-Langeheine

References

[1] W.A. Challener et al.: “Heat-assisted magnetic recording by a near-field transducer with efficient optical energy transfer”, Nat. Photonics **3**, 220–224 (2009), doi:10.1038/nphoton.2009.26

[2] J. Jensen, R. Allan: *Rare Earth Magnetism: Structures and Excitations* (Mackintosh Clarendon Press, Oxford, 1991)

[3] J.J. Rhyne and A.E. Clark: “Magnetic anisotropy of terbium and dysprosium”, J. Appl. Phys. **38**, 1379 (1967), doi:10.1063/1.1709631

[4] S.I. Anisimov, B.L. Kapeliovich, T.L. Perel’man: “Electron emission from metal surfaces exposed to ultrashort laser pulses”, Zh. Eksp. Teor. Fiz. **66**, 375377 (1974)

[5] J.K. Lang, Y. Baer, P.A. Cox: “Study of the 4*f* and valence band density of states in rare-earth metals: II. Experiment and results”, J. Phys. F: Met. Phys. **11**, 121 (1981), doi:10.1088/0305-4608/11/1/015

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Probing stimulated X-ray Raman scattering using photon recoil imaging

Ulli Eichmann, Max Born Institute, Germany

Non-linear processes have changed the way we look at the interaction between light and matter and have inspired the development of numerous optical techniques. Transferring these concepts into the X-ray regime—one of the driving forces behind the development of high-intensity X-ray FELs—would ideally allow us to explore the ultrafast coherent evolution of electronic wave functions in molecules, an ultimate, long-standing dream of non-linear X-ray physics. An essential building block to achieve this goal is the demonstration of stimulated X-ray Raman scattering (SXRS) using intense pulses from an X-ray FEL. We have proposed photon recoil imaging (PRI) as a new method to reveal and detect fundamental processes in the X-ray regime on the level of individual atoms. The experimental protocol allows detection of the scattered neutral atoms rather than the scattered photons. In one of the first user experiments at the SQS instrument of the European XFEL, we have successfully implemented the PRI method to demonstrate SXRS.

The control and the manipulation of quantum dynamics in atoms and molecules by means of short and intense photon pulses are two of the most fundamental and practically important applications of laser spectroscopy, for which numerous techniques have been developed. With the advent of X-ray FEL radiation, a central goal has been to merge the merits of X-ray spectroscopy, especially its ability to probe atom-specific local electron dynamics, with non-linear optical techniques [1].

Among important non-linear X-ray phenomena is the fundamental two-photon SXRS near an inner-shell resonance, which is crucial for the development of any non-linear X-ray method [2]. So far, stimulated emission and stimulated Raman scattering have been observed in dense media by measuring the scattered X-ray radiation [3]. The mandatory dense target, however, makes it cumbersome to separate the two-photon stimulated Raman scattering from stimulated processes initiated by the spontaneous radiative decay of core hole excited states. Moreover, since the stimulated light is inherently emitted in the forward direction, which coincides with the path of the driving X-ray laser beam, identification of stimulated Raman scattering using X-ray detection techniques is *per se* largely impeded.

Instead of using X-ray detection methods, we introduce PRI, which exploits the fact that the photon momentum transfer to the atom can be detected [4]. This allows for distinguishing the spontaneous X-ray Raman scattering, which is accompanied by a large momentum transfer to the atom, from SXRS, where the momentum transfer is almost negligible.

In our experiment at the SQS instrument, we used the core resonances of neon (Ne) [5] as a showcase to demonstrate that PRI can indeed be used to monitor SXRS on the single-atom level. SXRS leaves the Ne atom in an excited state, which further decays radiatively to a long-lived metastable state (Ne*). Such an excited metastable neutral atom can be directly detected using a multichannel plate (MCP) detector. The energy bandwidth of the European XFEL pulses is large enough to ensure SXRS.

We expanded the experimental capacities of the SQS instrument by adding a position-sensitive MCP detector, which was placed downstream of the collimated, pulsed atomic Ne beam (Figure 1a). The detector is sensitive to atoms with internal energy only, and the energy and momentum transfer during the scattering event, which takes place in the interaction volume (~1 cm x 1–2 μm diameter), is reflected in a corresponding deflection of the flight path of the atoms. The travel time of the atoms to the detector is about 350 μs. Thus, the velocity change of the atoms of 14 m/s after absorbing or emitting one photon results in a measurable deflection on the detector of about 5 mm (Figure 1b). In contrast, in the stimulated Raman scattering, the net momentum transfer to the atom is nearly zero, and the pattern of the excited neutral atoms impinging on the detector reflects merely the projection of the interaction volume (Figure 1b).

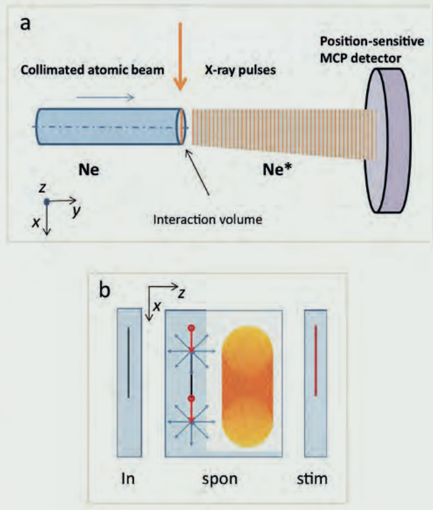


Figure 1: Principle of the experiment. (a) Experiment setup to detect metastable Ne* atoms and their deflection with a position-sensitive MCP detector. (b) Possible projections of deflected atoms from the interaction volume on the detector. Left (In): Projection of the mere interaction volume (black line). Centre (spon): Ne* pattern after spontaneous Raman scattering (right side). Scheme of the Ne* deflection: Absorption of an X-ray FEL photon causes photon momentum in the forward direction (red arrows), followed by isotropic momentum transfer after spontaneous X-ray photon emission (blue arrows). Right (stim): The Ne* pattern after stimulated Raman scattering is a mere projection of the interaction volume (red line).

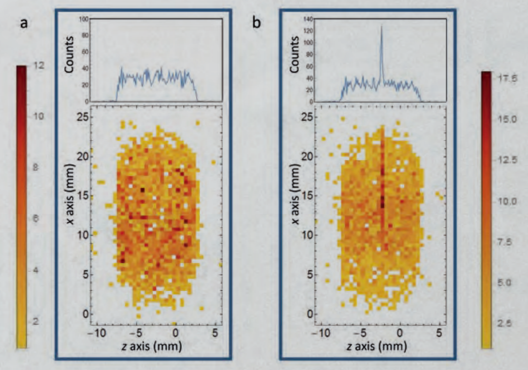


Figure 2: Distribution of Ne* atoms deflected as a result of momentum transfer during spontaneous X-ray Raman scattering. (a) At an incident photon energy of 860 eV. The upper panel displays the projection of the Ne* yield onto the *z* axis. (b) Same as (a), but at an incident photon energy of 855 eV. The additional narrow stripe of enhanced Ne* originates in SXRS. The projection in the upper panel clearly shows a peak due to SXRS.

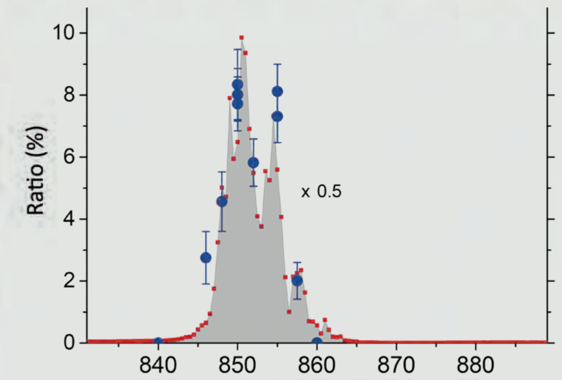


Figure 3: The ratio Ne^*_{stim}/Ne^*_{spon} from theoretical data (small red squares) compared with the ratio Ne^*_{stim}/Ne^*_{spon} (blue points) determined from the experimental yields.

Figure 2 shows typical detector images at two selected X-ray photon energies. At the first photon energy (Figure 2a), the distribution of detected atoms expected for spontaneous Raman scattering is clearly visible. Changing the photon energy to a value where stimulated Raman scattering should become more important, an additional pattern corresponding to SXRS arises. It can be clearly seen as a "vertical" line in the 2D pattern in Figure 2b and a corresponding spike in the projection. We scanned the incident X-ray photon energy over the range where the additional pattern is visible and determined the ratio of Ne* atoms produced by stimulated versus spontaneous Raman scattering (Figure 3). To explain the observation quantitatively, we solved a density matrix comprising the important atomic levels using the temporal electric field strength evolution of simulated X-ray FEL pulses. The experimental data are in very good agreement with the experiment, establishing PRI as a valuable tool to explore non-linear X-ray physics.

As an outlook, we envision to apply this method to SXRS in small molecules, such as carbon monoxide (CO). Furthermore, we are looking forward to the upcoming two-colour mode of the European XFEL, which will allow more well-defined and time-controlled SXRS experiments, for which PRI will be particularly fruitful.

Authors
U. Eichmann, H. Rottke, S. Meise, J.-E. Rubensson, J. Söderström, M. Agåker, C. Såthe, M. Meyer, T.M. Baumann, R. Boll, A. De Fanis, P. Grychtol, M. Ilchen, T. Mazza, J. Montano, V. Music, Y. Ovcharenko, D.E. Rivas, S. Serkez, R. Wagner, S. Eisebitt

References

[1] S. Mukamel et al.: "Multidimensional attosecond resonant X-ray spectroscopy of molecules: Lessons from the optical regime", Annu. Rev. Phys. Chem. **64**, 101–127 (2013), doi:10.1146/annurev-physchem-040412-110021
[2] V. Kimberg et al.: "Stimulated X-ray Raman scattering – a critical assessment of the building block of nonlinear X-ray spectroscopy", Faraday Discuss. **194**, 305–324 (2016), doi:10.1039/C6FD00103C
[3] C. Weninger et al.: "Stimulated electronic X-ray Raman scattering", Phys. Rev. Lett. **111**, 233902 (2013), doi:10.1103/PhysRevLett.111.233902
[4] U. Eichmann et al.: "Photon-recoil imaging: Expanding the view of nonlinear X-ray physics", Science **369**, 1630 (2020), doi:10.1126/science.abc2622
[5] A. Müller et al.: "Photoionization of Ne atoms and Ne⁺ ions near the K edge: Precision spectroscopy and absolute cross-sections", Astrophys. J. **836**, 166 (2017), doi:10.3847/1538-4357/836/2/166

Mapping the electronic structure of transient atomic states

Tommaso Mazza[1], Markus Ilchen[1,2], Michael Meyer[1]
[1]European XFEL, Germany
[2]Institute of Physics, University of Kassel, Germany

In this study of non-linear processes, which was one of the first user experiments performed at the SQS instrument, we used the ultrashort high-intensity X-ray pulses from the European XFEL to map the electronic structure of transient atomic states, capturing a snapshot of the short-lived state before its electronic decay. The experiment was realized by first creating a hole in the electronic core of a neon atom through absorption of an X-ray photon and then directly interrogating this excited system within its ultrashort lifetime of 2.4 fs by means of a second X-ray photon. With these investigations, it was possible, for the first time, to directly address such short-lived states, which critically determine the dynamics of the subsequently evolving system. Our results show that it is possible to efficiently control and independently probe excitations of specific electronic subshells at the SQS instrument. Experimentally addressing these elusive structures can help to validate the latest theoretical treatment of complex transient states in their role as mediators of photoinduced processes. The excellent agreement between experiment and theory is very promising to support advanced applications in physics, chemistry, and biology.

The universe is full of ionic matter for many reasons, one of them being the abundance of X-rays in space. The first step to generate an isolated ion is typically the process of photoabsorption, which is normally followed within extremely short times, i.e. within femtoseconds or shorter, by relaxation processes and the emission of one or more electrons. Exploring how such a highly energy-loaded and highly transient system looks before it relaxes is of great importance for many areas of X-ray physics, including investigations of ultrafast atomic and molecular processes. To this end, we have investigated, for the first time, the electronic structure of a neon atom directly after absorption of an X-ray photon, before its ultrafast decay.

For our experiments, we used the X-ray beam from the SASE3 undulator of the European XFEL, which provides, every second, an unprecedentedly large number of intense flashes of photons in the soft-X-ray wavelength range.

When X-rays interact with atomic neon, they most efficiently remove an electron from the electronic core level, which is labelled 1*s*, thus producing a highly excited ionic state (Figure 1, top left). This state typically decays by an electronic transition, in which an electron from the outer electronic levels (labelled 2*s* and 2*p*) fills the core hole while releasing the excess energy; this energy is predominantly transferred to yet another electron of the outer shells, which is ejected and leaves the atom doubly ionized (Figure 1, bottom). This process is called Auger decay. Auger processes are widely investigated in atoms, molecules, and solids because the emitted electron carries information about the electronic structure of the system.

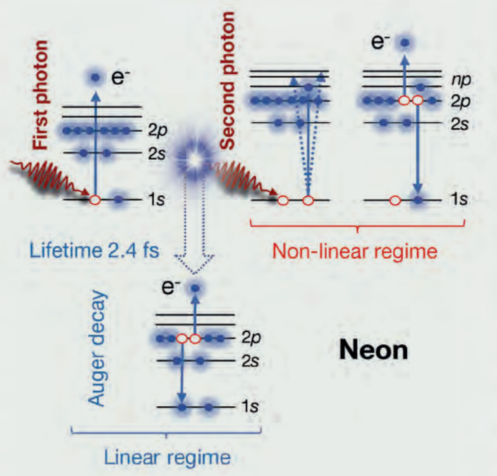


Figure 1: Scheme of the investigated process. Left: Linear regime. The first photon absorption and resulting ionization of neon is typically followed by an Auger decay after approximately 2.4 fs (from top to bottom). Right: Non-linear regime. With short pulses of sufficiently high fluence, this sequence can be intercepted by a second photon that creates Rydberg states in the transient ion. The relaxation of this double-core hole results in the ejection of an electron, which is the subject of the present investigation.

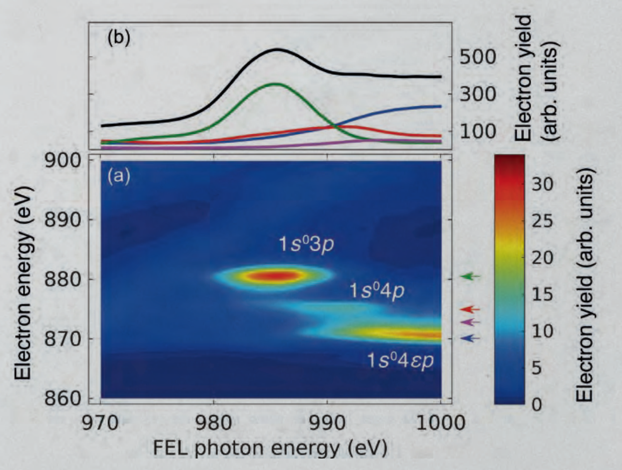


Figure 2: Resonance map of the transient neon ion. (a) Interpolated false-colour representation of the electron spectra recorded by varying the photon energy across the region of the DCH resonances in steps of 1 eV. (b) Total DCH Auger electron yield (black line). The total yield is decomposed into individual contributions for the different Rydberg states by projecting the 2D map at selected electron energies (see coloured arrows on the right side of (a)).

The European XFEL X-ray photons are delivered in pulses of a few femtoseconds' duration. With the very large number of photons within each single pulse, it is possible that a second X-ray photon from the same pulse can interact with the excited atom before the Auger decay occurs, i.e. within its lifetime of about 2.4 fs. In our study, the energy of the second photon was tuned to transfer the core electron to an unoccupied energy level, called a Rydberg state (labelled *np*, with $n > 2$). The photons have the right frequency to match the energy difference between the Rydberg states and the core level, thus creating a resonant double-core hole (DCH) in the transient ion. This DCH state relaxes in turn by emitting an Auger electron (Figure 1, top right). The energy distribution of this Auger electron carries the fingerprint of the electronic structure of the core-ionized transient state, which is effectively probed by the second X-ray photon.

This energy distribution is represented in a false-colour plot in Figure 2. The figure shows the kinetic energy spectra of the DCH Auger electrons emitted by tuning the photon energy across the Rydberg resonances. Each column in the map (line of pixels in the direction of the *y* axis) is an electron spectrum taken at a different photon energy: States are generated in which two holes are induced in the core and one electron is in a Rydberg level, labelled $1s^0np$, with $n > 2$. The decay of these states is characterized by specific electron energy distributions.

The comparison of the experimental results, discussed in detail in Ref. [1], with theoretical calculations allows for a detailed characterization of the decay pathways of these highly excited resonant states and for an estimation of the relevance of the different contributing channels. It is instructive to compare the contribution of the different channels with what is observed in the counterpart resonant Auger decay for the neutral neon atom, which can be investigated at synchrotron sources [2]. Compared to single-core hole resonances, differences are observed in the relative weight of specific contributions, which can be interpreted as a difference in the spatial distribution of the electron wave functions in the transient core-excited ion compared with the neutral system. The electron spectroscopy of the DCH Auger decay thus indeed gives access to the electronic fingerprint of the transient short-lived state.

Taking advantage of the high intensity and the high number of X-ray pulses delivered to the SQS instrument at the European XFEL, we were able to demonstrate the possibility to perform a spectroscopic analysis of short-lived intermediate states. The promising results open a new and alternative way to investigate fast electronic processes, which are important for many chemical and biological reactions.

Authors

T. Mazza, M. Ilchen, M.D. Kiselev, E.V. Gryzlova, T.M. Baumann, R. Boll, A. De Fanis, P. Grychtol, J. Montaño, V. Music, Y. Ovcharenko, N. Rennhack, D.E. Rivas, Ph. Schmidt, R. Wagner, P. Ziolkowski, N. Berrah, B. Erk, P. Johnsson, C. Küstner-Wetekam, L. Marder, M. Martins, C. Ott, S. Pathak, T. Pfeifer, D. Rolles, O. Zatsarinny, A.N. Grum-Grzhimailo, M. Meyer
Publication: Ref. [1]

References

[1] T. Mazza et al.: "Mapping resonance structures in transient core-ionized atoms", Phys. Rev. X **10**, 041056 (2020), doi:10.1103/PhysRevX.10.041056
[2] A. Kivimäki et al.: "Auger decay at the 1*s*–1*np* (n = 3–5) resonances of Ne", J. Electron Spectrosc. Relat. Phenom. **114**, 49 (2001), doi:10.1016/S0368- 2048(00)00259-0

Realizing a two-colour pump–probe setup at the SASE3 undulator

In a close collaboration between DESY and European XFEL, a major upgrade of the soft X-ray branch of the facility was realized with the installation of a magnetic chicane in the central part of the SASE3 undulator. The device allows the introduction and control of a temporal separation of up to 2.5 ps between the femtosecond X-ray pulses generated in the first and second section of the undulator, respectively, by delaying the electron bunches in the chicane. In addition, the photon energy of the X-ray pulses can be independently selected in the individual undulator sections, and energy differences of several hundred electronvolts can be realized. This two-colour operation mode with adjustable temporal delay and photon energy offers the unique possibility to perform time-resolved X-ray pump / X-ray probe studies at the soft X-ray instruments SCS and SQS. The magnetic chicane was installed during the summer shutdown of 2020, and first time-resolved experiments at the SQS instrument demonstrated the successful operation of the two-colour pump–probe (2CPP) setup.

An essential part of the science scope of the European XFEL involves time-resolved investigations. In particular, pump–probe experiments are used to gain insight into the temporal evolution of a system after photoexcitation. In these studies, a first photon (pump) excites the system and triggers a process, such as the fragmentation of a molecule, and the second photon (probe) interrogates the evolving system after a well-controlled and variable time delay. In most cases, these studies are based on the combination of ultrashort X-ray pulses with pulses of a synchronized optical laser. A more profitable scenario is realized by using two X-ray pulses. Soft X-ray pulses in particular allow for addressing one specific atom in the sample, i.e. it is possible to excite a molecule at a specific atomic site and to probe the influence of the excitation at another site. The 2CPP setup [1] thus offers unique opportunities to study the dynamics of various fundamental processes, such as charge migration, photoinduced changes in the molecular geometry, or fragmentation processes.

In order to realize the 2CPP setup at the soft X-ray SASE3 undulator, a magnetic chicane was added in the middle of the undulator (Figure 1a). The chicane consists of four 60 cm long dipoles and delays the electron beam by up to 2.5 ps at a beam energy of 8.5 GeV and up to 0.75 ps at 17.5 GeV. Negative delays can be accessed using an optical delay line (Figure 1b), to be installed at a later time, or by applying the so-called fresh-slice method, which involves tilting the beam transversely in the undulators [1].

The design of the chicane is similar to that for the hard X-ray self-seeding setup at SASE2 and fits into the 5 m space required for one undulator segment. To maximize the obtainable delay, the field strength of the four bending magnets of the chicane was roughly doubled by increasing the length of the magnets. The magnets were designed and built at the Efremov Institute in St. Petersburg, Russia. A special vacuum chamber (Figure 2) was designed by the DESY vacuum group. It allows both for a large beam offset

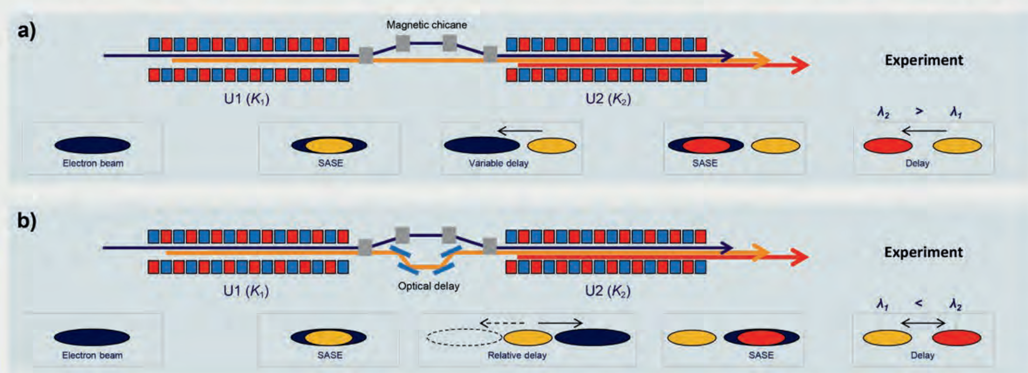


Figure 1: Two-colour scheme at the SASE3 undulator. (a) Setup realized in 2020 with a four-bounce magnetic chicane in the middle of the undulator. (b) Possible upgrade with an optical delay line in parallel to the magnetic chicane (from [1]). U = undulator section; K = undulator strength parameter; λ = X-ray photon wavelength.

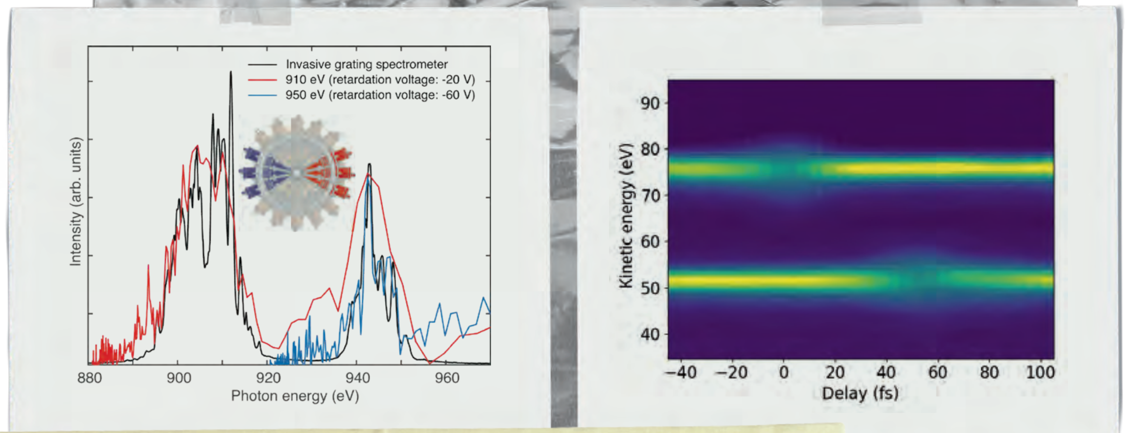


Figure 3: Characterization of the 2CPP setup at SASE3. Left: Single-shot electron spectra of neon with the PES optimized for photon energies of 950 eV (blue line) and 910 eV (red line), emitted in the undulator sections U1 and U2, respectively. Single-shot spectra of the photon pulses measured with a grating spectrometer are shown as a black line. The inset shows the 16 eTOF drift tubes of the PES oriented perpendicularly with respect to the X-ray beam, with different subsets optimized for the different photon energies. Right: Electron spectra for C1s ionization of CH_3F for photon energies of 688 eV (upper line) and 662 eV (lower line). The X-ray pulses are separated in time by 50 fs, visualized by the perturbation in the electron spectra due to the overlap with the optical laser pulse.

of up to 48 mm created at maximum delay and for straight beam passage. All four bending magnets are powered by a single power supply. The chicane is controlled in a manner similar to that of the SASE2 self-seeding chicane, allowing the operators to set either the magnetic field strength or the calculated beam offset, or delay.

The SASE3 undulator typically allows the generation of an X-ray pulse energy of about 1 mJ with only half of the 21 segments (first undulator section U1). The remaining undulator length and electron beam quality can be used to emit another radiation pulse of different “colour” (second undulator section U2). The X-ray pulse duration is determined by the electron beam lasing window and is typically on the order of 30 fs. For specific pump–probe experiments, this can be reduced either by lowering the electron bunch charge or by employing the fresh-slice method. For monitoring the soft X-ray pulses, the SASE3 photoelectron spectrometer (PES) is employed as a non-invasive pulse-resolved diagnostic device, consisting of 16 electron time-of-flight (eTOF) drift tubes oriented perpendicularly to the X-ray beam (insert in Figure 3, left). Hardware modifications were undertaken to enable independent tuning of the retardation voltages for different subsets of eTOF drift tubes in order to optimize the resolution at different photon energies. Figure 3 (left) shows typical eTOF spectra of atomic neon recorded with the PES, with the undulator sections U1 and U2 tuned to 950 eV and 910 eV photon energy, respectively. This data set was collected in single-bunch mode, allowing a direct comparison to the data measured simultaneously by the invasive grating spectrometer.

The full performance of the 2CPP setup was tested at the SQS instrument by studying the photoionization of fluoromethane (CH_3F) molecules. Photoelectron spectra following carbon inner-shell (C1s) ionization were recorded

Figure 2: Installation of the chicane in the tunnel. The 60 mm wide vacuum chamber is inserted in the four bending magnets. The complete structure is mounted on a single steel and concrete girder.

in the presence of an additional optical laser. By means of the fresh-slice method, it was possible to generate a 688 eV pump pulse with an average energy of 600 µJ and 15 fs FWHM duration, followed by a 662 eV probe pulse with an average energy of 1200 µJ and comparable duration. Different delays were realized using the chicane and visualized with the overlapping optical pulses, demonstrating the successful operation of the new SASE3 2CPP setup (Figure 3, right).

The realization of the 2CPP setup, which was installed and commissioned in a strong collaborative effort by a number of different groups from DESY and European XFEL, was enabled thanks to financial support by the Academy of Finland. The setup will be available for users in 2021.

Authors

This article summarizes the contributions from different groups from DESY (MXL, MVS, MEA, and MKK) and European XFEL (FPH, XPD, XO, TS, UND, PMO, and SQS).

Reference

[1] S. Serkez, W. Decking, L. Fröhlich, N. Gerasimova, J. Grünert, M. Guetg, M. Huttula, S. Karabekyan, A. Koch, V. Kocharyan, Y. Kot, E. Kukk, J. Laksman, P. Lytaev, T. Maltezopoulos, T. Mazza, M. Meyer, E. Saldin, E. Schneidmiller, M. Scholz, S. Tomin, M. Vannoni, T. Wohlenberg, M. Yurkov, I. Zagorodnov, G. Geloni: “Opportunities for two-color experiments in the soft X-ray regime at the European XFEL”, Appl. Sci. **10**, 2728 (2020), doi:10.3390/app10082728

NEWS AND EVENTS

Opening the ultra high-speed data connection between European XFEL and NCBJ

News and Events

29–31 January
Record attendance at Users' Meeting

With more than 1300 participants from 28 countries, the 2020 DESY and European XFEL Users' Meeting was the largest convention of its kind worldwide. Participants met in Hamburg for three days of discussion about research and developments at the state-of-the-art light sources in the area: DESY's X-ray sources PETRA III and FLASH as well as the European XFEL. The main user meetings were complemented by 20 satellite meetings and workshops, a presentation of more than 400 scientific posters, and an industrial fair with more than 80 suppliers of scientific equipment and technical solutions.

11 February
International Day of Women and Girls in Science

11 February marks the International Day of Women and Girls in Science. Alongside its partners at EIROforum, European XFEL celebrated this day by sharing stories of female colleagues working in STEM professions and by arranging a get-together.

18 February
Shaping attosecond waveforms

An international team of researchers led by Guiseppe Sansone from the University of Freiburg in Germany and including scientists from European XFEL have, for the first time, been able to reliably generate, control, and characterize attosecond light pulses from a free-electron laser. Chemical reactions and complex phenomena in liquids and solids are determined by the movement and rearrangement of electrons. These movements occur on an extremely short time scale, typically only a few hundred attoseconds (1 as = 10^{-18} s or one quintillionth of a second). Light pulses of comparable duration can be used to take snapshots of the dynamics of electrons. The results, which published in the journal *Nature*, open up new approaches for controlling electronic dynamics in real time.

19 February
EU and Russia strengthen scientific cooperation

Research institutes from the EU and Russia, including European XFEL, will cooperate even more closely in the future. Thirty-five partners have joined forces in the EU project CREMLINplus, coordinated by DESY, 10 of them from Russia and 25 from the EU and associated countries. In the kick-off meeting at DESY with about 100 representatives of the participating institutions, the Russian Ministry of Research announced in-kind contributions worth 15 million euro for the project. The EU is funding the four-year project with 25 million euro within its Horizon 2020 research framework programme.

19 March
Super laser delivered to European XFEL

The high-repetition-rate, high-energy laser DiPOLE 100-X was delivered to European XFEL. Developed in the UK at the Central Laser Facility (CFL) of the Science and Technology Facilities Council (STFC), it is part of the UK contribution to the HiBEF user consortium. The laser will be used at the HED instrument of the European XFEL to generate extreme temperatures and pressures in materials. Related picture was taken in January 2020.

3 April
The art of science

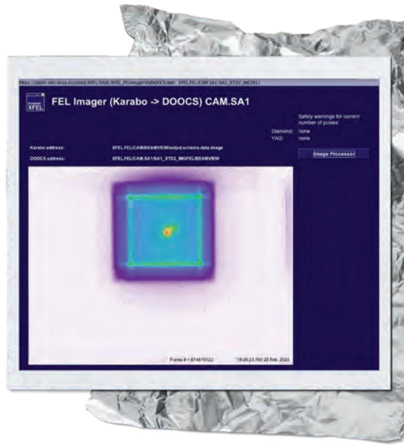
A new webpage was launched that details the art projects initiated, commissioned, and supported by European XFEL. Over the years, the facility has supported independent artists to realize their projects portraying the life and spirit of European XFEL and has worked with artists to present the science happening at European XFEL in inspired ways.

7 April
European XFEL and FAIR sign collaboration agreement

In a video link between Hamburg and Darmstadt, representatives from European XFEL and the international accelerator Facility for Antiproton and Ion Research (FAIR) signed a collaboration agreement. Within the framework of the Memorandum of Understanding, FAIR and European XFEL will share best practices, knowledge, and results and exchange experiences in areas such as administration and user support. Furthermore, the organizations aim to build on synergies in industrial cooperation and promote scientific and technological results for the benefit of society.

8 April
European XFEL reaches world-record photon energies

With a photon energy of 25 keV, corresponding to a laser wavelength of 0.05 nm, DESY's operations team for the European XFEL accelerator set a new wavelength record for laser light. Furthermore, by changing the setting of the undulator SASE1 — one of the light generation devices of the European XFEL — to 30 keV, the accelerator team was able to push the limit even further, observing clear indications of free-electron laser radiation.



The availability of femtosecond pulses of hard X-rays opens up unprecedented scientific opportunities to probe matter and materials at the atomic scale on ultrashort time scales. With its unique capability to generate intense X-ray pulses at energies of 25 keV and beyond, the European XFEL enables the possibility to delve into unchartered worlds and study complex phenomena like never before.

16 April
Virtual tour of the European XFEL online

With the updated virtual tour, science and technology fans can take a walk along parts of the European XFEL tunnel system, starting from the accelerator control room on the DESY campus, to the experiment stations in the underground experiment hall in Schenefeld. Guests may even explore parts of the facility that are no longer accessible, such as the electron dump in Osdorfer Born.

The tour consists of high-resolution 360° photographs of a total of 51 different locations within the facility, combined with short and concise explanations of the components and instruments.

24 April
X-ray science facilities contribute to overcoming COVID-19

X-ray science facilities worldwide, in a remote-access video summit on 23–24 April, adopted an action plan to further coordinate and strengthen their support of scientific research on and solutions to the COVID-19 pandemic. The aim of the international network of X-ray synchrotron radiation and free-electron laser facilities is to create and implement scientific and technological research activities to effectively study, understand, and contribute solutions to the COVID-19 pandemic, including new drugs, therapeutic strategies, and medical equipment developments.

7 May
European XFEL contributes to COVID-19–related research

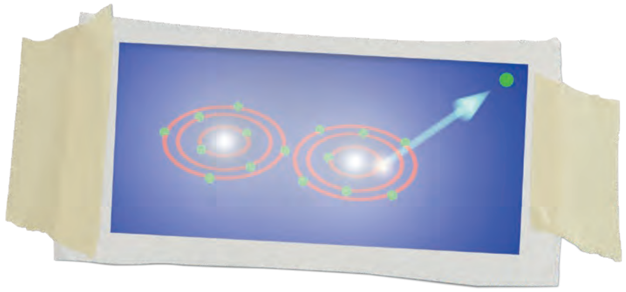
European XFEL contributes to the global campaign against the novel SARS-CoV-2 coronavirus by facilitating research related to COVID-19. X-ray light can provide insight into the virus that may help to develop therapies to treat the disease. European XFEL is equipped with state-of-the art laboratories and technologies. After six weeks in reduced operation mode, European XFEL restarted operation of the X-ray laser in early May. Although regular user operation was not yet possible, proposals for COVID-19–related research at the instruments and laboratories were being sought. In the course of the year, the biolabs contributed to three projects, ranging from basic to application-orientated research.

7 May
European XFEL celebrates guest house topping-out ceremony

On 7 May, European XFEL celebrated its topping-out ceremony of the guest house on the Schenefeld campus. Due to the corona measures, the celebration was limited to a small circle of participants. European XFEL Managing Director Nicole Elleuche thanked the construction team for their commitment. The guest house will mainly accommodate external users, who usually come to Schenefeld for one week to conduct their experiments.

9 June
Snapshots of exploding oxygen

An international collaboration of scientists led by Till Jahnke from Goethe University Frankfurt in Germany succeeded in observing the ultrafast breakup of single oxygen molecules. The proof-of-concept experiment was carried out at the soft X-ray SQS instrument at the European XFEL and demonstrated the great potential of using photoelectron diffraction for imaging small molecules.

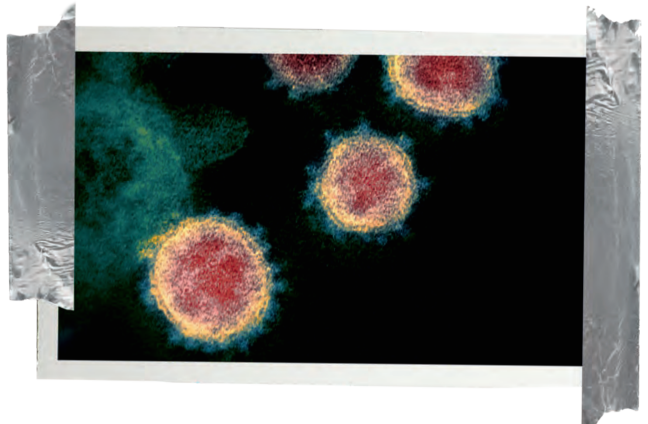


12 June
Ultrahigh-speed data connection to Poland opens

Secretary of State Wolf-Dieter Lukas of the German Federal Ministry of Education and Research (BMBF) and Undersecretary of State Grzegorz Wrochna of the Polish Ministry of Science and Higher Education opened an ultrahigh-speed connection for the exchange of scientific data between the two countries. The new connection between European XFEL, DESY, and National Centre for Nuclear Research (NCBJ) in Otwock-Świerk near Warsaw will be used to analyse data from experiments carried out by international teams of researchers at the European XFEL.

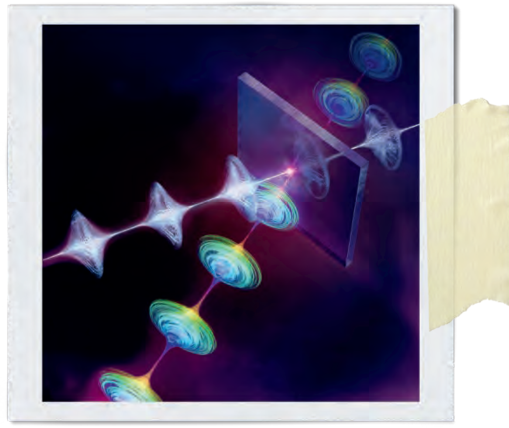
15 June
Open science COVID-19 analysis platform online

As part of the EU-funded project PaNOSC, an international network of data scientists developed the Open Science COVID Analysis (OSCOVIDA) platform to analyse the spread and development of COVID-19 cases across the world. The interactive platform offers plots of COVID-19 cases to better understand the development of the disease on different time and geographical scales. The data is collected from a number of renowned national sources. Higher-resolution data is also available from some regions, such as for 412 districts in Germany and the individual states in the USA.



16 June
First megahertz-rate timing jitter observed

Scientists at the SPB/SFX instrument of the European XFEL demonstrated accurate synchronisation of optical and X-ray lasers, which is crucial for pump–probe experiments at X-ray FELs. In such experiments, a precisely synchronized optical laser is used to trigger a reaction, while the X-ray laser takes a snapshot of the molecular structure at defined times during the reaction. These snapshots are then stitched together to make molecular movies. For such experiments to be successful, the “timing jitter” between the synchronized lasers must be kept to a minimum and be accurately characterized. At SPB/SFX, scientists succeeded in achieving the lowest ever mega-hertz-rate timing jitter (24 fs with an uncertainty of 12.4 fs). This enables experiments working with time intervals upwards of 100 fs to be performed without requiring extra measurements or analysis to take the jitter into account.



19 July
Maria Faury to continue as Chair of the European XFEL Council

At the European XFEL Council meeting held on 18–19 June, Maria Faury was re-appointed Chair of the Council, and Martin Meedom Nielsen was re-appointed Vice Chair. The Council is the highest governing body of European XFEL and functions as the shareholders’ assembly, deciding on important issues of the company and the X-ray laser facility.

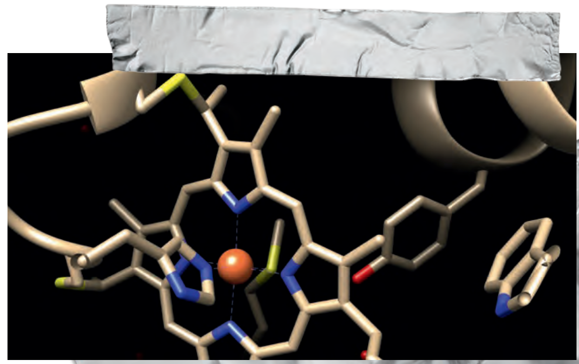
14 August
Visitor centre plans are to take shape

European XFEL finalized the first tenders for its visitor and conference centre by awarding a contract to the architectural firm DBCO GmbH in Münster, Germany. The architects convinced the jury with their innovative design for a new building featuring an exhibition, school laboratories, and seminar rooms, which will be built on the European XFEL campus in Schenefeld. The exhibition-planning contract was awarded to Archimedes Exhibitions GmbH in Berlin. The start of construction is planned for 2021.

The new visitor centre will provide an opportunity to learn about the world’s largest X-ray laser and the research performed there. An interactive exhibition of 350 m^2 will be complemented by tours and events. School students will carry out hands-on experiments in physics and biochemistry in two school laboratories. In addition, seminar rooms will be available for scientific conferences, workshops, and public events.

1 September
Unlocking secrets of two vital proteins

Scientists used the FXE instrument of the European XFEL to reveal hidden secrets of two proteins that are vital for proper cellular functioning: nitrosyl-myoglobin and cytochrome c. The international team of scientists that carried out the study was led by researchers from École polytechnique fédérale de Lausanne (EPFL), Switzerland, in collaboration with scientists from Japan, the UK, Poland, and European XFEL.



2 September
User operations restart

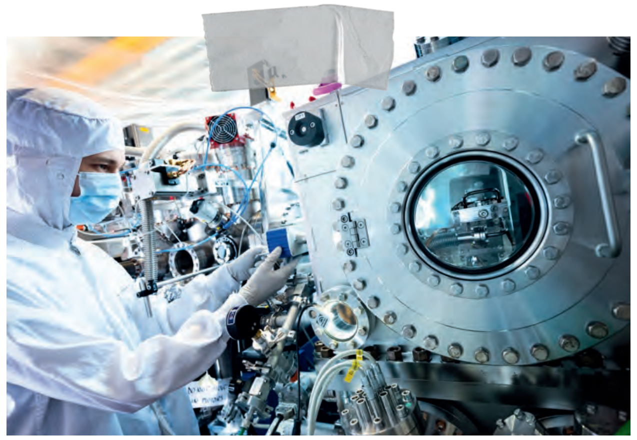
After around six months of reduced operation due to the COVID-19 pandemic, European XFEL restarted user experiments at the beginning of September. Fewer users than usual were on site, with a majority participating in the experiments remotely. In previous runs, around 30 experiments were usually scheduled, but, due to COVID-19–related restrictions, only 16 experiments were slated for this run. All six European XFEL instruments were in operation. Alongside rapid-access COVID-19–related research, the selected experiments covered a wide range of topics, some of which directly addressed societal challenges, such as studying environmentally friendly crop protection options by determining the structure of bacterial insecticides, or gaining deeper insights into vitamins important for metabolism, such as coenzyme B12, by understanding the ultrafast changes in its electronic structure.

11 September
New technique reduces sample volume and waste

A research team comprising scientists from Arizona State University in the USA and European XFEL developed a unique technique that can dramatically reduce waste of precious biological samples. This paves the way to structural analysis and molecular movies of substances that are difficult to isolate in larger quantities. The team also revealed new details of a protein that has an important function in gram-negative bacteria, with potential applications for the development of new antibiotics. The results of this new approach were published in *Nature Communications*.

14 September
Science@FELs goes online

The fifth edition of the Science@FELs conference, this year jointly organised by DESY and European XFEL, took place online on 14–16 September with over 700 registered participants. The meeting is organized biannually by the FELs of Europe collaboration and has evolved into one of the most important international conferences for FEL science. The 2020 programme covered a broad range of topics, including imaging, materials science, femtochemistry, bioscience, and laser physics. The talks were complemented by two poster sessions and three focus tutorials in which young scientists had the chance to learn more about particular topics from established scientists.

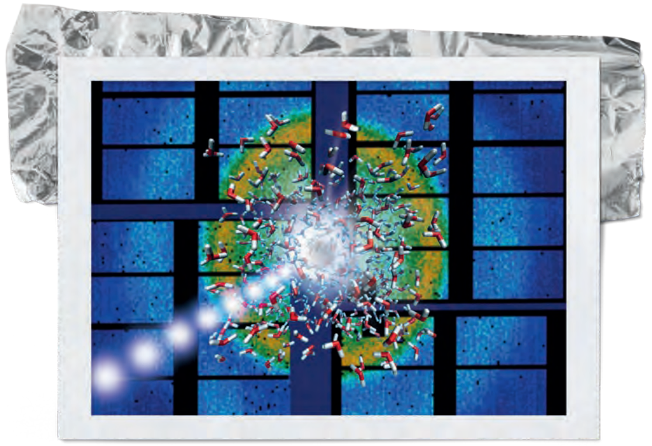


15 September
Accurate temperature snapshots

A team of scientists, with lead researchers from SLAC National Accelerator Laboratory in the USA, Oxford University in the UK, and European XFEL, established methods to accurately measure temperature in rapidly evolving, transient systems. This is important for diverse purposes, such as developing materials for spacecraft thermal shields, which face extreme changes in temperature and pressure when re-entering the Earth's atmosphere, or studying the interior of giant planets such as Jupiter, Saturn, Uranus, and Neptune. The results are based on the data obtained from the very first beamtime and user experiment held in 2019 at the HED instrument of the European XFEL.

16 September
Surprising behaviour of superheated water

The essence of an ideal tool for gaining deeper insights into soft-matter physics, biology, or nanoscience is to accurately capture changes and movements that occur in a sample within microseconds, while maintaining the integrity of the sample. At the SPB/SFX instrument of the European XFEL, a team of scientists used a method called X-ray photon correlation spectroscopy on a sample of silica nanospheres dispersed in water. They demonstrated that the technique can be used to capture the microsecond-quick changes, even in heat-sensitive and delicate samples.

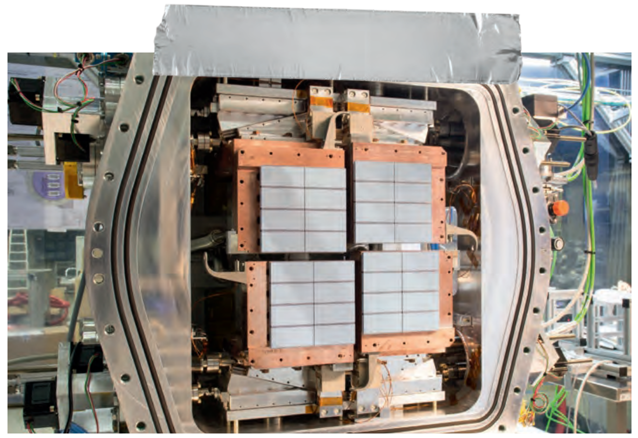


17 September
New avenues for solution-phase chemistry

A team of scientists used the FXE instrument of the European XFEL to shed light on photoexcited polynuclear metallogrid complexes—that is, molecular complexes containing several transition metal ions. Photoabsorption causes the electronic and magnetic properties of such molecular complexes to undergo profound alterations, which can be traced back to ultrafast spin flips at the metal ion centres. Using femtosecond X-ray emission spectroscopy, the scientists revealed that such metallogrids possess unexpected properties, which make them particularly interesting for a relatively new field of science—spin-driven photochemistry in the solution phase.

22 September
ATTRACT reveals how research can ignite a deep tech revolution

ATTRACT is a Horizon 2020 research and innovation project funded by the European Union and backed by a consortium of nine partners, including European XFEL. In 2019, it had announced 170 breakthrough ideas that would each receive 100 000 euro to develop sensing and imaging technologies to change society. A new study by CERN in Switzerland, Esade Business School in Spain, and the Technical University of Denmark shows that conditions for serendipity in science and technology can be created by forming innovation ecosystems where serendipity is somehow systematized—leading to streamlined scientific breakthroughs that ignite deep tech innovation in Europe. These findings, based on a large data set from the above-mentioned 170 technologies developed within the ATTRACT project, were presented at the ATTRACT conference, "Igniting the Deep Tech Revolution", held on 22 September.

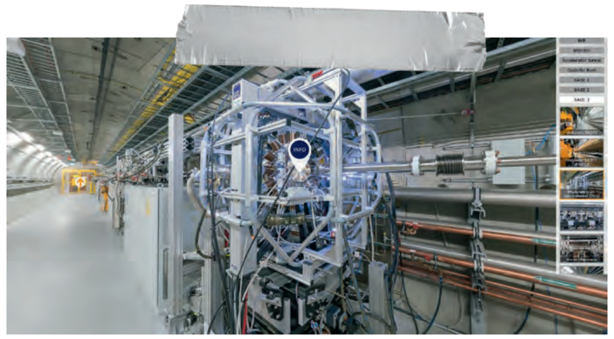


24 September
2020 FELs of Europe award for Rebecca Boll

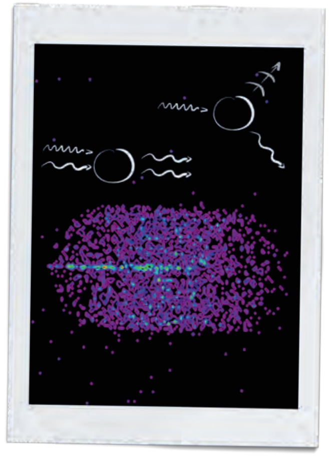
Rebecca Boll, a scientist in European XFEL's SQS group, was awarded the 2020 FELs of Europe award on FEL science and applications. The award recognizes her outstanding research on multiple ionization of rare gases and photoinduced dynamics of ring-type molecules. European XFEL Scientific Director Serguei Molodtsov presented the award to Boll in a virtual award ceremony during the Science@FELs conference.

25 September
Course on X-ray FELs for master and Ph.D. students expands

The joint lecture course “Materials Research at X-Ray Free-Electron Lasers” organized by European XFEL and TU Bergakademie in Freiberg, Germany, was expanded in 2020 to also involve master and Ph.D. students from other institutions, including the universities of Hamburg and Kassel. Usually held in Hamburg, the intensive block course, which ran from 21 to 25 September, was conducted in an online format for the first time. With over 100 participants, the online format proved to be a good way to open up the course to a larger number of students.



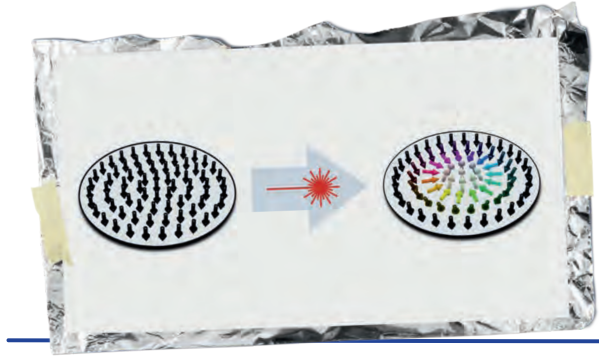
25 September
A new approach to look inside molecules



A German–Swedish research team with lead authors from Max Born Institute in Germany, Uppsala University in Sweden, and European XFEL investigated what happens when an intense X-ray beam crosses paths with a supersonic jet of atoms, using a new method called photon recoil imaging. They found that they could identify single atoms that underwent a rare process known as stimulated Raman scattering. The results, which were obtained at the SQS instrument of the European XFEL and published in *Science*, pave the way towards controlling the motion of electrons in an atom or a molecule. This could be used for the efficient manipulation of atoms and molecules to gain a deeper understanding of fundamental physics or for practical applications, for instance in batteries and solar cells.

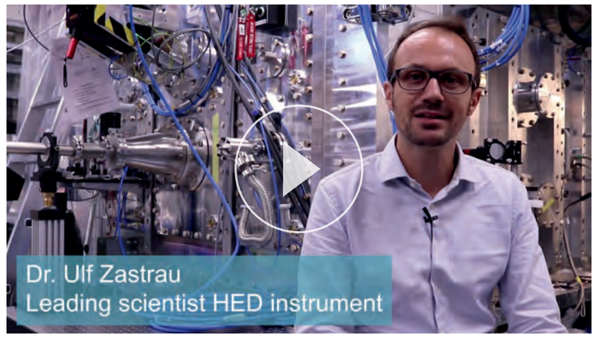
7 October
Controlling tiny magnetic swirls in the sea of spins

Skyrmions, commonly imagined as tiny magnetic swirls, are nanoscale magnetic quasi-particles that have recently become a hot topic because of their potential in the development of faster and more effective data storage devices. For the first time, an international group of scientists, with lead scientists from the Massachusetts Institute of Technology in the USA and the Max Born Institute in Berlin, were able to observe the formation of skyrmions in a magnetic material using ultrashort laser pulses, shedding light onto the microscopic process and its time period. The X-ray pulses of the European XFEL revealed the creation of tiny skyrmion structures on nanometre length scales at a speed that is faster than previously thought possible.



21 October
Video series on European XFEL instruments

In a new video series, leading European XFEL scientists take online visitors on a virtual tour of their instruments. The series contains videos for expert and non-expert audiences. In the shorter version, the scientists address a wide audience, and experts can tune in to the longer version to get more in-depth information.

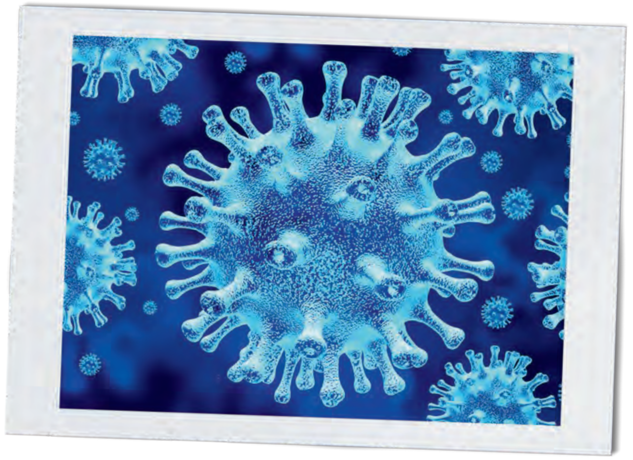


18 November
LGBTQ+ STEM Day 2020

18 November is the International Day of LGBTQI+ People in Science, Technology, Engineering, and Maths (LGBTQ+ STEM Day) to raise awareness and show support for the LGBTQI+ in STEM community. European XFEL values individuality and diversity and strives to ensure a positive and welcoming work environment where everyone, irrespective of religion, cultural background, gender, or sexual orientation, feels safe and is able to be themselves. In support of this day and the LGBTQI+ community, European XFEL raised the rainbow flag and encouraged colleagues to take part in virtual LGBTQ+ STEM Day events.

25 November
Lecture: X-ray vision aids search for corona drugs

An online public lecture held on 25 November by Kristina Lorenzen from European XFEL and Alke Meents from DESY gave insights into the details of viral proteins from the coronavirus SARS-COV-2. The speakers also explored a range of questions: How many drug candidates did the researchers find? How were the experiments validated? And can these substances slow down the reproduction of the virus?



26 November
DASHH graduate school receives North German Science Award

The graduate school DASHH Data Science in Hamburg – Helmholtz Graduate School for the Structure of Matter was awarded the North German Science Award 2020 (Norddeutscher Wissenschaftspreis), which comes with 125 000 euro in prize money. In the project, Universität Hamburg cooperates with numerous institutions from Hamburg and other northern German states, including European XFEL and DESY, to provide innovative training and cooperation for Ph.D. students in the field of data science.

8 December
X-ray laser in action

A safety test captured on video made for some fascinating tech viewing. The video shows the glowing nitrogen molecules that have interacted with the extremely intense X-ray beam of the European XFEL. This interaction has lit up the beam as it travels through the air, allowing a peek at X-rays that are otherwise invisible. The safety test was carried out by the safety staff and scientists from European XFEL and DESY at European XFEL’s SQS instrument.

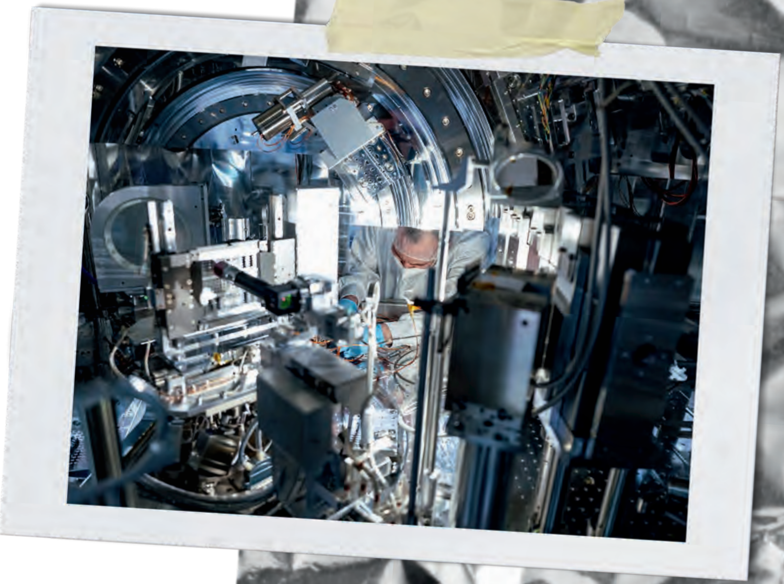
https://www.youtube.com/watch?v=_lnL4VMaioQ

19 December
Mapping out a transient atom

An international team from Germany, Sweden, Russia, and the USA, led by scientists from European XFEL, published the results of an experiment that could provide a blueprint for the analysis of transition states in atoms and molecules. This would open up new opportunities to gain insights into important processes, such as photocatalysis, elementary steps in photosynthesis, and radiation damage. In the first user experiment carried out at the SQS instrument of the European XFEL, the scientists used high-resolution electron spectroscopy to capture a snapshot of the short-lived transient state produced when X-rays punch a hole in the very core of the atomic electron cloud. The results of the study, which was carried out on neon atoms, are the starting point for the analysis of transient states.

MAGAZINE

A scene from the control hutch during an HED experiment



Making lasting (remote) connections

Remote work, smart work, virtual meetings, and Zoom calls became part of the common parlance in 2020 when the COVID-19 pandemic forced institutions across the world to rethink what "coming in to work" meant. European XFEL has been no exception, and many aspects of scientific and administrative work have been affected. The Management Board's and the Council Chair's forewords (pages 4, 5 and 7, respectively), the Director's outlook (pages 78,79), and the chapter on company development (page 66) reflect the (huge) impact of the pandemic. In 2020, European XFEL was supposed to enter smooth and full-fledged user operation as the facility had transitioned from construction to operation phase between 2017 and 2019. But when lockdowns came into effect in Germany, European XFEL had to quickly adapt to the new normal.

The decision to reduce staff on site, with most working from home, meant an immediate need for scalable IT and computing infrastructure solutions. Steve Aplin, head of the Data Department, and his team knew that the company needed to make quick decisions to ensure that every employee could seamlessly transition into a remote work mode. They selected a commercial solution as the main video conferencing tool after a risk–benefit assessment, which was quickly accepted by the staff and ensured the company stayed operational.

Ensuring staff could work from home during the lockdown was just one part of the story. As a user facility, the company had to develop an ecosystem that could support operations for user-led experiments carried out remotely for the second user run in the fall of 2020. Staff scientists, technicians, engineers, and the support groups who were on site had their work cut out for them. "For experiments to have the highest chances of success, we had to provide the users with access to as much information as possible so that they could participate in the decision-making process and decide the next steps in the remotely controlled experiments," explains Sakura Pascarelli, Scientific Director at European XFEL. "And in case of remote user operations, this meant maintaining a close connection with users who were not on site, throughout a number of days and across different time zones," she adds. "Our teams ensured that users could access images from optical cameras installed in the control and experiment hutches, the data and analysis software, and live detector images," she says.

Because the pandemic and the travel restrictions worldwide had made remote user access for all experiments the general rule, very few users were present on site in 2020. "We could only authorize presence of users on site after reviewing a detailed written request from the main experiment proposer," says Silvia Bertini, Head of the User Office. "The users who could come on site had to undertake a specific online COVID-19 hygiene training, and we ensured that we had relayed the latest government regulations from travelling from risk areas and possible quarantine measures," she adds. For staff and users on site, there have been strict regulations in place. The occupancy of instrument hutches, user laboratories, meeting rooms, middle zone offices in the main building,

Figure 1: Staff members sport the European XFEL-branded masks, which were distributed between July and December 2020.

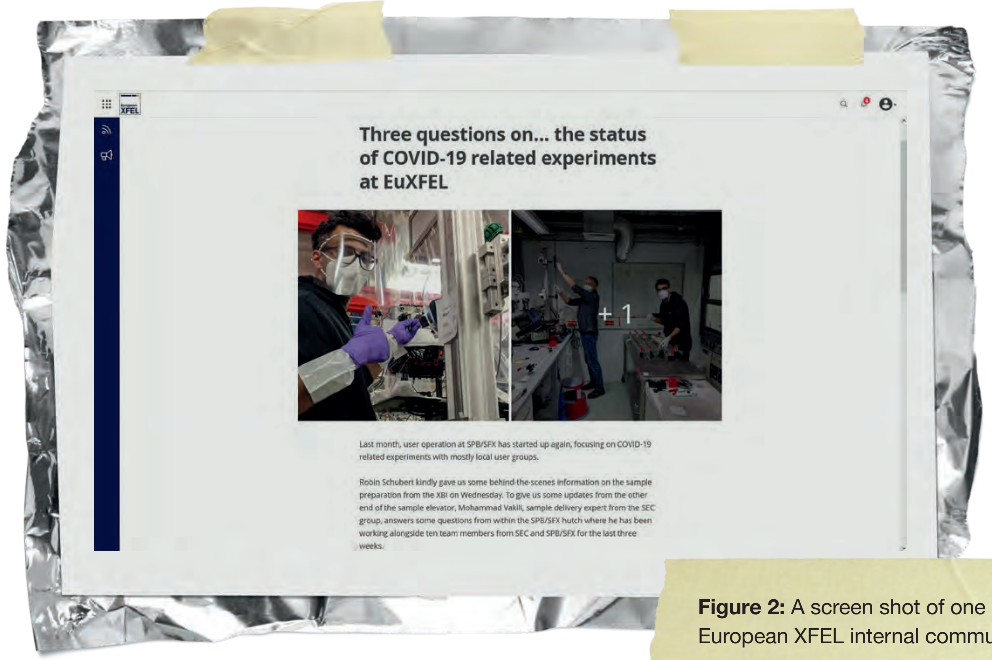


Figure 2: A screen shot of one of the posts on the European XFEL internal communications channel.

and other public areas have been limited. Tasks, such as those performed in control and experiment hutches, that require working at close distances have been only allowed with FFP2/KN95 masks provided by the instrument teams.

The efforts to stay connected extended beyond running the facility and the experiments. “Our company has had a strong tradition of holding monthly meetings to which all staff is invited,” says PR officer Marieke Sander, who coordinates Internal Communications. When the first lockdown in March 2020 was announced, this tradition was quickly adapted for an online version and continued. The Internal Communications team, which includes members of the Human Resources (HR) and Press and Public Relations (PR) groups, had been considering the idea of setting up a new and interactive internal news platform. “The idea was to be able to post internal news more quickly than in the monthly email internal news bulletin,” says Sander. “The pandemic accelerated this development, and in August, after thorough trial phases and with the support and advice from Legal, IT, Procurement, and Archiving colleagues, we launched our internal communications platform, where all colleagues are encouraged to publish and share news. It has proven to be a great connector across our various groups,” Sander adds.

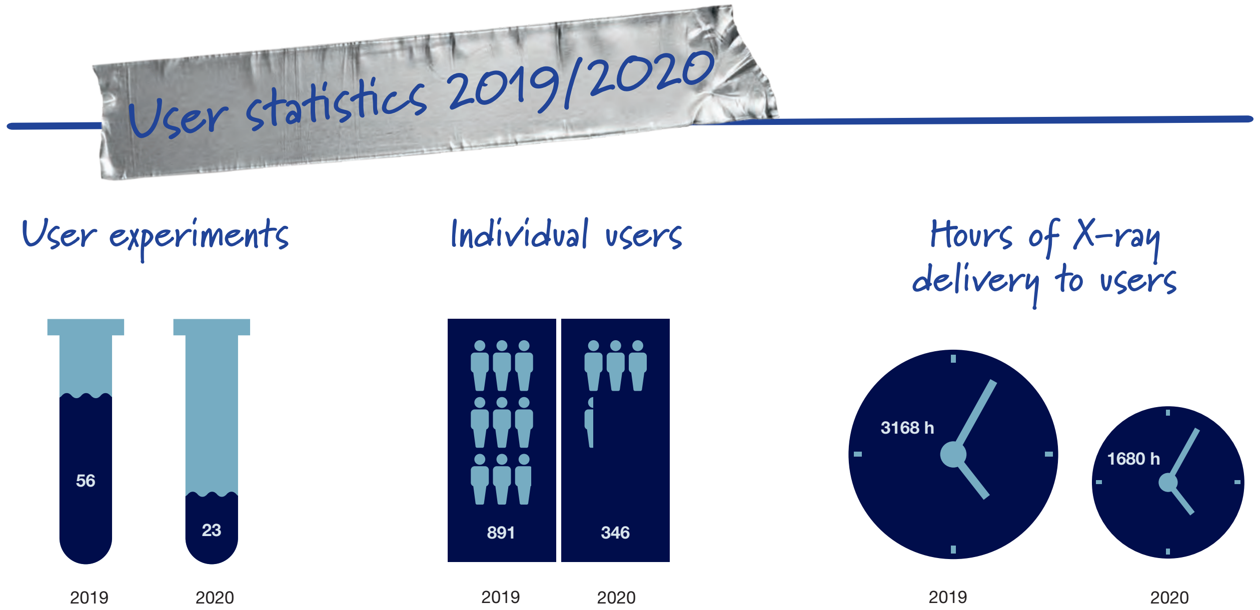
The HR group had to meet other hurdles. European XFEL is a growing company, and this means regular recruitment drives and dealing with candidates from outside Germany and even Europe. “The biggest challenge for us arose when the international travel restrictions affected newly recruited colleagues from abroad. At times, embassies were unable to issue visas due to pandemic-related travel restrictions, and in some cases, new colleagues had to start their work remotely from their home country, and as a result international taxation and social insurance rules proved to be big hurdles,” says Wolf-Ulrich Sauermann, head of the HR group. “And, once the colleagues arrived, we faced the challenge of integrating them into the company culture. Our virtual welcome days were much appreciated—however, nothing replaces the face-to-face encounters,” he says.

While there is a sense of eagerness to see how things unfold and how much we can go back to as it was earlier, lessons learned and some procedures adopted will endure. European XFEL has been agile in adapting to the new normal while continuing to work on experiments, including drug screening for combating the coronavirus and experiments aimed at getting better insights into the virus structures. The close collaboration across the company ensured that research would go on in the face of the pandemic. “In a way, the pandemic has forced our hand in enhancing the capabilities for doing remote analysis in real time,” says Aplin. “In the future, scientists won’t have to necessarily travel to European XFEL to take an active part in the online analysis of the experiment,” he points out. “We will learn to reduce travel with more remote connections. The way we organize meetings, conferences, and workshops will change,” adds Pascarelli. “I think that science and scientists in general will come out of this crisis strengthened.”

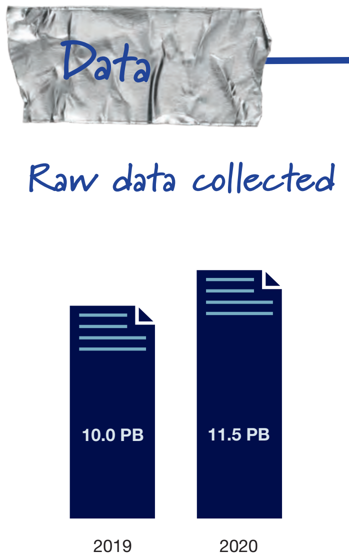
Factsheet

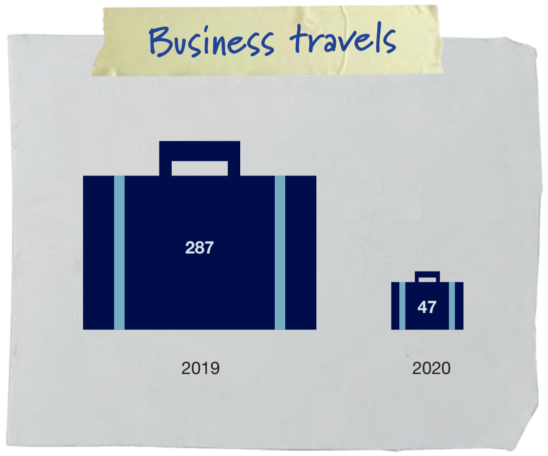
The comparison shows how experiments and the amount of data collected have been impacted by the shift to remote work due to COVID19.

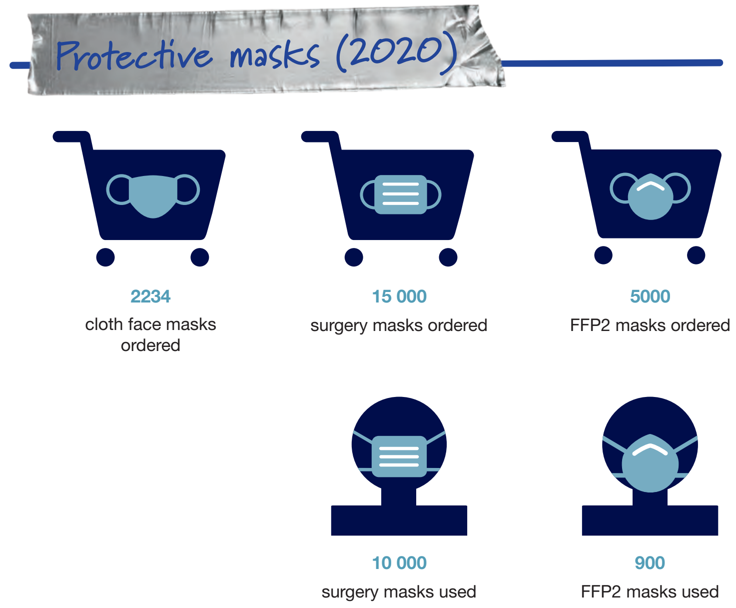
User statistics 2019/2020

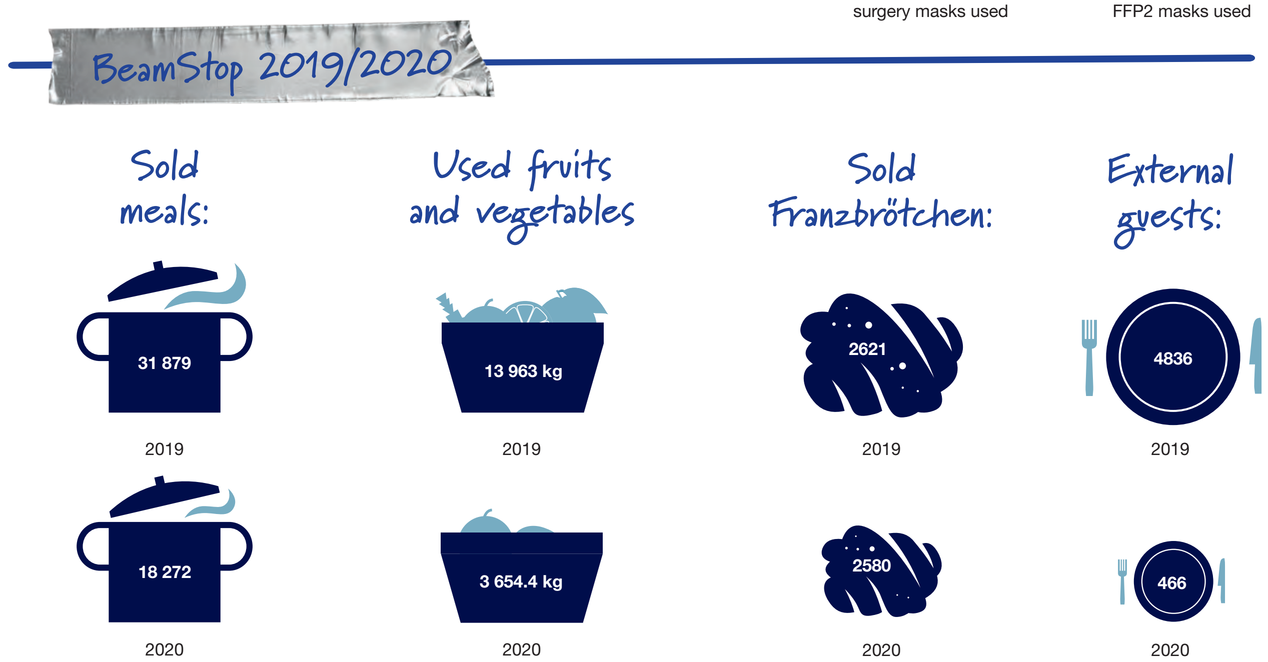


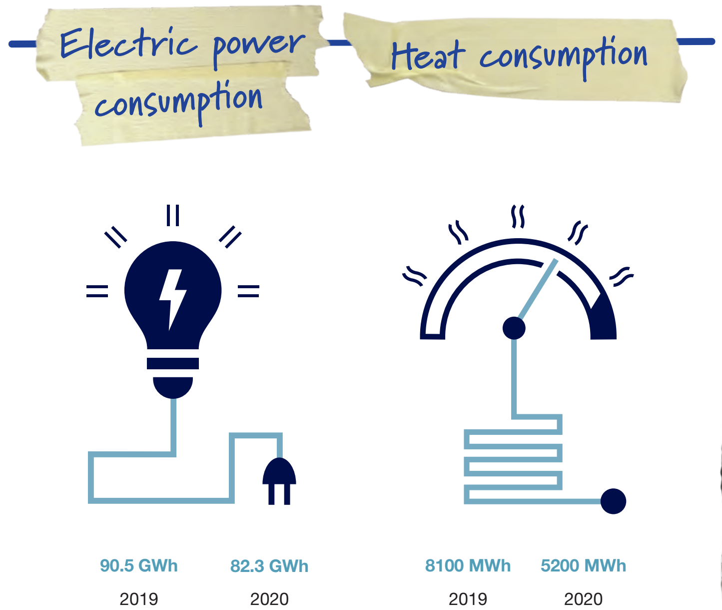
Data

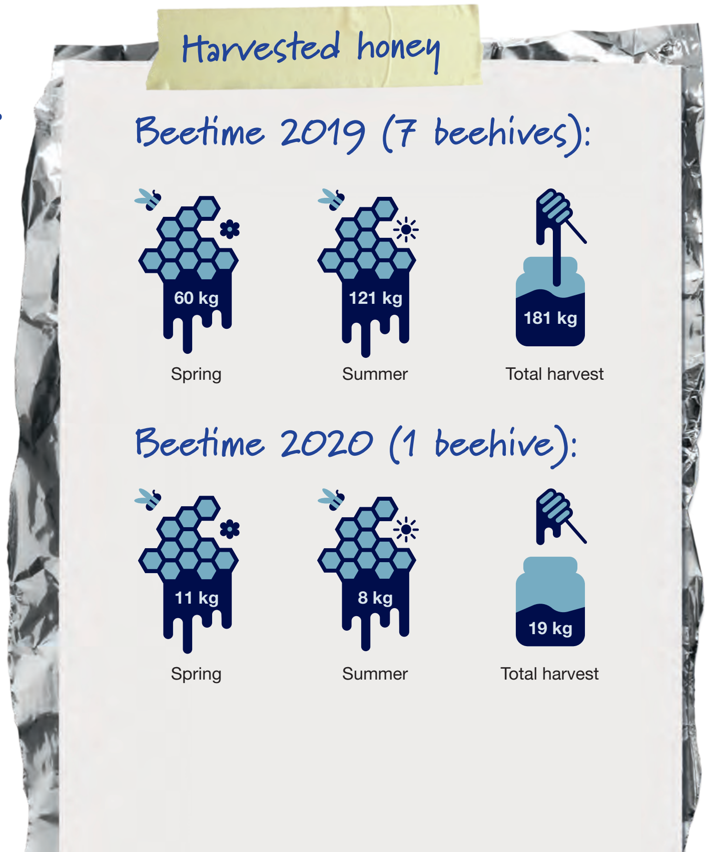












OPERATIONS

At the control hutch for an MID experiment before the lockdown

Operations

While operation in 2020 was restricted by the COVID-19 pandemic and the original operational goals for all accelerator, FEL, and experiment systems could not be reached, many other milestones were achieved. The performance of the SASE2 FEL was improved, enabling pulse energies similar to those at SASE1, and the installation of a magnetic chicane in SASE3 allowed first “two-colour” pump–probe experiments with photon pulses of two different wavelengths created from the same electron bunch. Two additional electron energy working points of the accelerator at 11.5 and 16.5 GeV extended the range of photon energies delivered to the experiments, and operation at reduced bunch charge allowed shorter X-ray pulses. The scientific instruments successfully switched to remote operation and, from July to November, user experiments were performed at all six instruments, including a few selected through a rapid-access programme for research addressing COVID-19.

According to the original operation plan for 2020, which foresaw a total of 6888 h scheduled for accelerator operation, 3144 h would have been dedicated to X-ray delivery (Figure 1). After the winter shutdown of 2019–2020, the accelerator was successfully restarted, followed by a three-week period of X-ray delivery. During this time, an availability of 90% was achieved, meaning pulse energies above a defined threshold could be provided. Problems with stable delivery were encountered, in particular at the SASE2 FEL, leading to reduced availability. During those three weeks, most of the scientific instruments used the X-ray beam for commissioning and setup, with only four user experiments scheduled and conducted as of mid-March. By then, however, the COVID-19 pandemic had significantly affected most countries and the experiments suffered from travel restrictions, which hindered users from participating on site.

In mid-March, the European XFEL Management Board and the DESY Directorate decided to shut down the European XFEL accelerator and take precautions to avoid irreparable damage in case of failure of supporting infrastructure, such as the cryogenic and water cooling systems, during lockdown times, when service personnel would not be able to access the facility. This precautionary measure required a mechanical detuning of the approximately 800 cavities, a procedure that was intended for use only in case of a warmup of the helium-cooled accelerator. This enforced accelerator shutdown lasted from 20 March to 10 May. During this time, installation and maintenance work that had originally been planned for the summer shutdown was carried out. Work in the tunnels was performed with reduced staff, applying protective measures and distancing rules.

Following the easing of restrictions, the accelerator was restarted on 10 May with an operation concept relying on extended remote support by experts to minimize the presence of staff members. The scientific instruments were carefully restarted, with still greatly reduced staff on site, and without X-ray beam delivery to the instruments. During this time, a period of approximately two weeks was dedicated to improving the performance of the SASE2 undulator. It was possible to achieve pulse energies at SASE2 similar to those at SASE1, which could be maintained throughout the second half of 2020.

The regular summer shutdown from 8 June to 3 July could not be shortened or rescheduled due to contractual commitments for work by external companies as well as the mandatory annual interlock test. Preponing activities

Operating hours

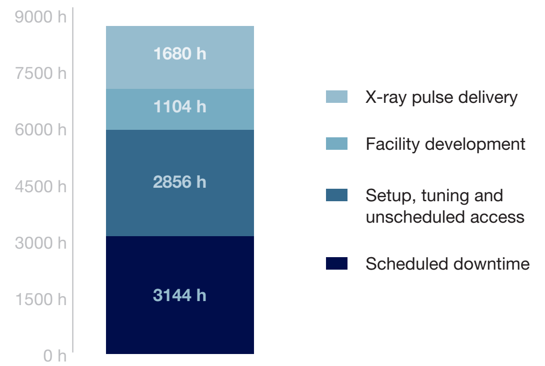


Figure 1: Operating hours of the European XFEL accelerator in 2020. The cryogenic system of the accelerator was operated throughout the entire year (8784 h). Finally, 1680 h were provided for X-ray delivery, 1104 h for facility development, and 2856 h for setup, tuning, and unscheduled access. The remaining 3144 h were scheduled downtime.

SASE FEL performance

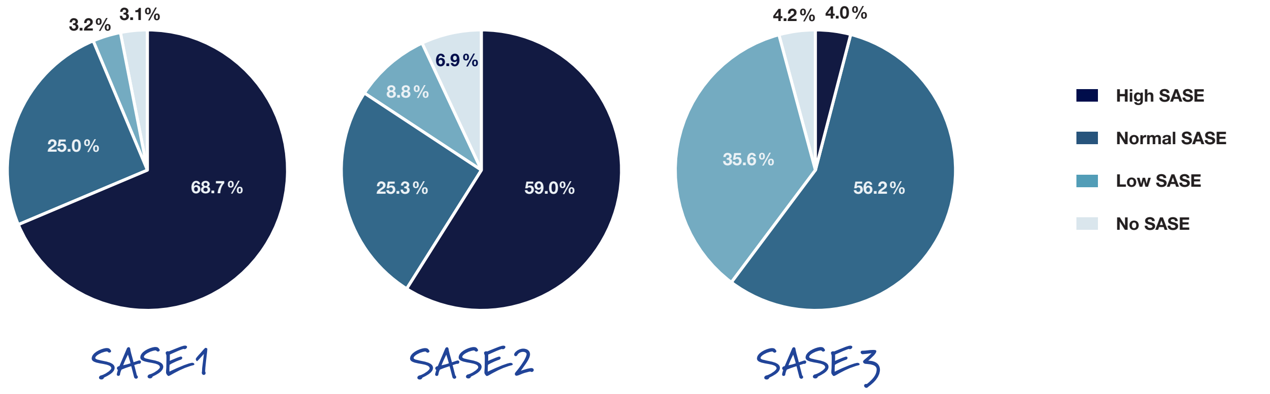


Figure 2: Pulse energy statistics for the SASE1, SASE2, and SASE3 FELs achieved during X-ray delivery in the second half of 2020. The classification of the pulse energy performance (low, normal, or high SASE) depends on the FEL and the photon energy.

to the enforced shutdown reduced the workload during the summer shutdown, so that all planned maintenance and installation tasks could be completed, in particular the installation of a magnetic chicane in SASE3, which allows the control of the temporal delay between two photon pulses created from the same electron bunch (see chapter Technical Highlight).

Operation after the summer shutdown was initiated by the third restart of the facility in 2020. As a consequence, startup procedures had matured and become highly automated. In the second half of 2020, the European XFEL accelerator was operated without major problems and with very good performance overall. The operation schedule was adjusted, as the demand for X-ray delivery and the possibility to schedule user experiments were reduced due to the travel restrictions caused by the pandemic. Instead, facility development time was increased by about two weeks, which were mainly used to commission the hard X-ray self-seeding at SASE2 and the two-colour pump–probe setup at SASE3 as well as to improve longitudinal (timing) stability. An additional week for setup was included after the summer shutdown to accommodate the northern branch with the SASE1 and SASE3 FELs, which had not been operated since March. During this period, standard operation at an electron energy of 14 GeV was complemented by two weeks at 11.5 GeV and two weeks at 16.5 GeV. These two additional electron energy working points were used to extend the range of photon energies delivered to the scientific instruments. As another special mode, the accelerator was operated for about two weeks at a reduced bunch charge of 100 pC, which allowed a stronger compression of the electron bunches and therefore shorter X-ray pulses. In a total of 11 weeks of X-ray delivery after the summer shutdown, all scheduled shifts could be delivered and an average availability of 95% was achieved at all three FEL sources.

With the additional, enforced shutdown and the modified operation plan, a planned annual accelerator operation of 5640 h was achieved, which included 1680 h for X-ray delivery and 1104 h for facility development. An additional 2856 h were used for accelerator, FEL, and instrument setup as well as tuning, maintenance, repair, and other unscheduled access (Figure 1). In 2020, the time required for the latter mode was significant, as it included the three facility startup procedures after the regular winter shutdown, the enforced shutdown, and the regular summer shutdown as well as the two-week period for tuning of SASE2. The remaining 3144 h in Figure 1 are the sum of the originally scheduled and enforced downtimes.

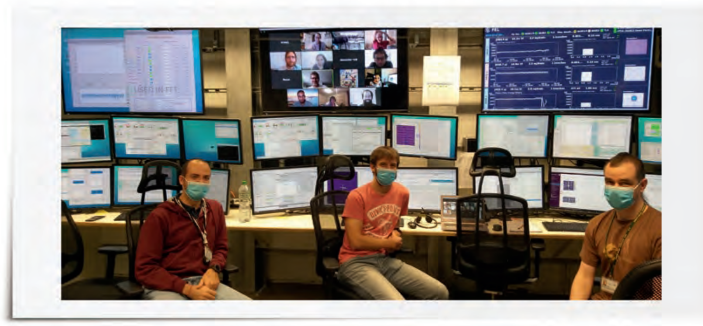


Figure 3: User operation in times of travel restrictions: The user groups participated in the experiments through videoconference tools and remote data access.

The planned winter maintenance period started at the end of November. In addition to maintenance and repair work, major activities included the modification of about 30 m of the electron beam transport system behind SASE3 and the installation of additional programmable kicker magnets to improve the compensation of eddy current effects in the electron beam distribution system.

X-ray operation in 2020 was largely limited to the time after the summer shutdown. From July to November, the facility was run for a total of 11 weeks in X-ray delivery mode, during which continuous operation of the three FEL X-ray beam transport systems and the six scientific instruments was achieved (Figure 2). A total of 19 user experiments were performed during this time at the instruments, in addition to various internal activities for commissioning and research. The user experiments had to be conducted largely by the staff of the scientific instruments, with the user groups participating remotely (Figure 3). Only six users were on site during the entire second half of 2020. Remote operation of the instruments included videoconferencing, access to online data, use of video cameras, as well as near-online and offline data analysis. This mode of operation put a much higher load on the scientific instrument teams and was possible only for experiments that did not require very detailed expertise to perform the proposed measurements. On the positive side, users could focus on data analysis, thereby making the experiments more efficient and, in some ways, more successful.

The regular proposal review and user experiment allocation were also affected by the modified operation schedule and the travel restrictions for users. Most of the user experiments scheduled for the first half of 2020 had to be shifted. Some of these could be rescheduled to the second half of 2020 if they were feasible without the on-site presence of the user groups (Figures 4, 5, and 6). A similar strategy was applied to the high-ranked proposals reviewed in February 2020. Consequently, a significant backlog of approved user experiments developed, some of which could be postponed to the first half of 2021 and some of which had to be cancelled. In addition, the call for proposals in summer 2020 was cancelled, and only one call was performed at the end of 2020. This call led to a record number of nearly 170 submitted proposals.

In support of international activities to fight the pandemic, the European XFEL management initiated a rapid-access programme for experiments related to research addressing COVID-19. A call for expressions of interest for COVID-19–related research was published. Twenty expressions of interest were received and evaluated with the goal to define targeted experiment proposals.

Five groups of users were invited to submit COVID-19–related experiment proposals in a specific, restricted call. Following peer-review, one community proposal was allocated rapid access at the SPB/SFX instrument in November 2020, while two additional community proposals were set to receive beamtime at SPB/SFX in 2021.

Overall, the operation of the X-ray systems in 2020 was very smooth, and the activities of the newly formed X-Ray Operations group contributed to this efficient operation. In the first half of 2020, the group supported the general planning of activities during the reduced operation. After the restart, it facilitated remote user operation as well. From September, the group started preparations for the planning of the winter maintenance period, including closer support for the precise scheduling of work, the identification and resolution of resource conflicts, and the monitoring and scheduling of nearly 700 activities.

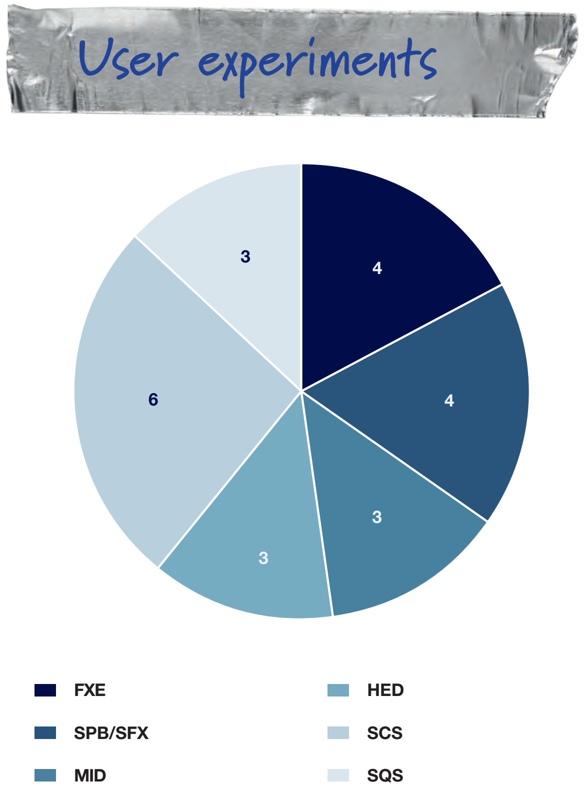


Figure 4: Number of user experiments allocated beamtime at the six scientific instruments in 2020

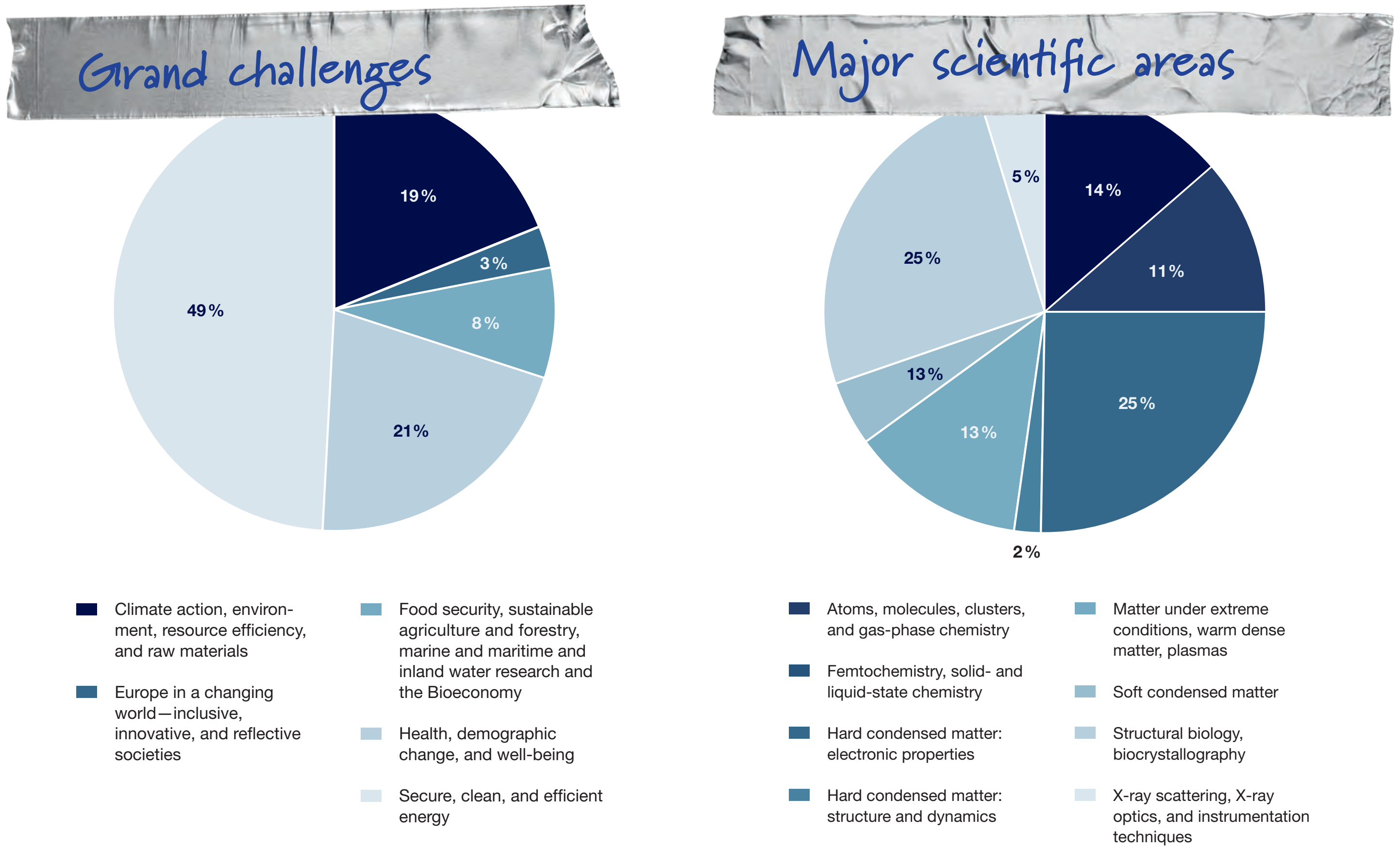


Figure 5: Distribution of users according to grand challenges (left) and major scientific area (right)

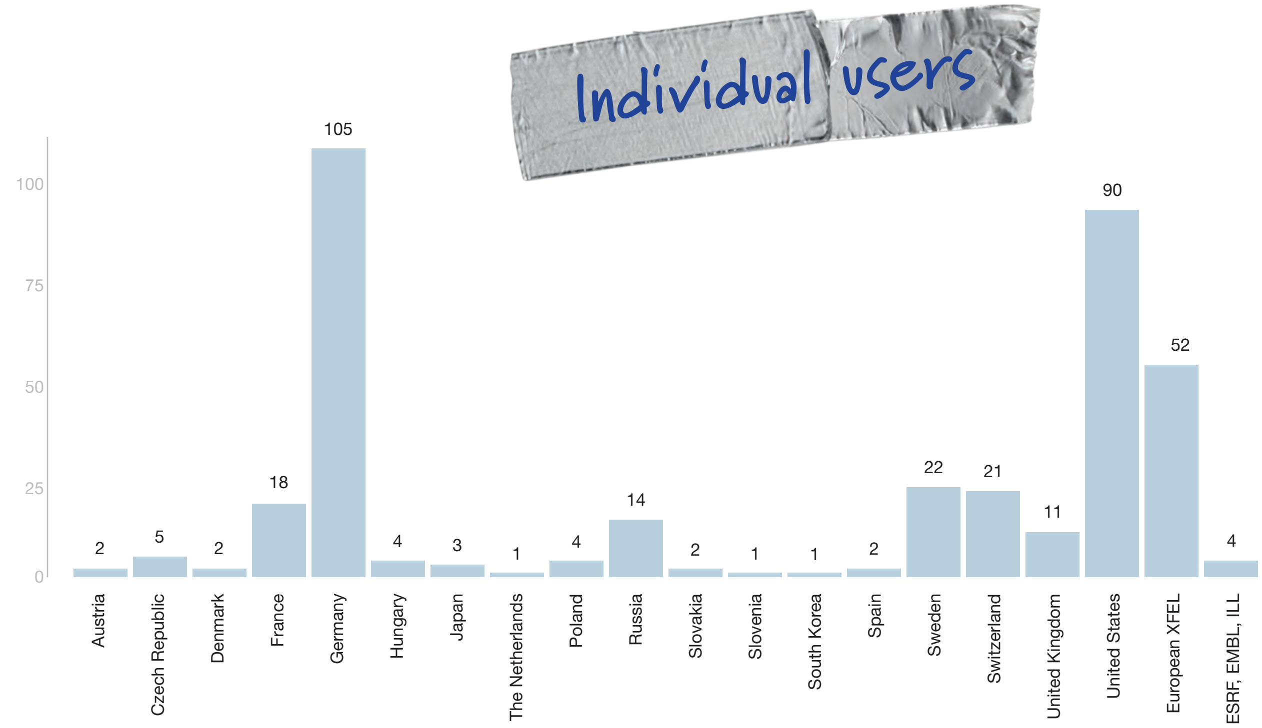


Figure 6: Distribution of individual users participating (mostly remotely) in experiments in 2020, shown by country of affiliation

FACILITY UPDATE

Aerial view of the European XFEL site in Schenefeld, including the planned buildings

Campus Development

The new undulator hall and the guest house, which were largely finished in 2020, will be home to new activities and facilitate life on the Schenefeld campus.

Despite general restrictions related to the COVID-19 pandemic, construction activities in 2020 continued at nearly full pace. This led to the near completion of the new undulator hall and guest house buildings, while other new installations for storing technical gases and dangerous materials advanced. Furthermore, preparations were made for the new office building and the visitor centre.

The undulator hall building was largely finished by the end of 2020 and will be handed over to the Undulator Systems group in February 2021. The building, which also includes a small workshop and offices, provides space for measuring magnetic structures, calibrating, and storing spare undulators as well as materials. The new magnetic measurement rooms have been built with a minimum of magnetic materials, in particular using carbon-reinforced concrete for their foundations and roof panels. After the transfer of the magnetic measurement benches from Hall 36 at DESY is completed in 2021, the availability of laboratories on the Schenefeld campus will entail a significantly reduced need for travel to DESY.

Considerable progress was achieved in the construction of the guest house. The outer shell and the façade were completed by the end of 2020, and the construction and technical infrastructure work inside progressed well too. On the north-side façade, a picture of Rosalind Franklin (1920–1958) was sculptured. (Rosalind Franklin was the first to interpret the X-ray diffraction pattern of DNA correctly, thereby giving evidence to what we know today as the double helix structure.) The guest house has 58 beds in 55 rooms and is expected to open its doors in the first half of 2021. It will enable users, committee members, guests, and visitors to stay on campus when visiting European XFEL. A new gate built next to the guest house will enable significantly shorter access to Metro Bus 1 as of June 2021.

During 2020, good progress was made in the construction of areas for technical gases and dangerous goods. The technical gas storage area was completed and will go into operation during the first months of 2021. Here, pressurized gases will be stored prior to their use in laboratories and experiments. In the area for dangerous goods, the foundation and paving are nearly ready for installation of five special containers for storing different types of dangerous goods and collecting them for disposal. Further activities were large-scale planting on the campus, landscaping the field above the underground tunnels, and installing information panels related to specific locations and buildings.

In addition, several improvements were made to the headquarters office building and laboratory floors as well as to the experiment hall. New offices were created for 14 persons in the headquarters building, and air-conditioning units were installed in the corridors on the south side. On the laboratory floor, a new room was created for electronic works, and additional racks were installed for electronics to be used in the laboratories. In the experiment hall, preparations were made for the power supply room of the high-field magnet supplied by the HiBEF user consortium to the HED instrument, and a station was built to handle hazardous liquids.

The campus will develop further with the new office building and the visitor centre. For the new office building, pre-planning was completed and the approval process was initiated. The call-for-tender procedure for construction is scheduled to start in early 2021, with the building expected to be available in the second half of 2022, finally providing adequate office space for all staff members currently housed in temporary buildings. For the visitor centre, the architecture competition was concluded, with a winning design by DBCO (Münster, Germany). The landmark building will complete the square formed by the restaurant, the headquarters office building, and the visitor centre, and will provide spaces for exhibitions, a cinema hall, school laboratories, versatile seminar and lecture halls, and offices for the operating staff. The approval process is expected to start in early 2021, and inauguration is planned for 2023.

Figure 1: Measurement hutches inside the new undulator hall. In them, the magnetic measurement of the undulator segments will be performed under well-defined thermal, vibrational, and magnetic field conditions.

Figure 2: Façade of the guest house showing the portrait of Rosalind Franklin, one of the pioneers in the structure determination of biomolecules.

Figure 3: Illustration of the new office building with office space for 200 persons. On the ground floor, next to the entrance, a lounge will provide work and relaxation space to visitors, guests, and staff members. Barrier-free access is possible, both on the ground floor and in the basement.

Figure 4: Winning design for the visitor centre, with the exhibition area on the ground floor and a flexible conference space for up to 320 persons on the first floor.

Figure 5: Schenefeld campus plan

Schenefeld campus plan showing the layout of existing buildings, those under construction, and those to be built in the near future

= completed = under construction or planned

A headquarters/experiment hall (XHQ/XHEXP), B BeamStop restaurant and cafeteria, C central electrical station (XHPSC), D pump station and cooling (XHPSC), E undulator hall (XHU), F tunnel entrance buildings (XHE2–4), G guest house (XHG, under construction), H dangerous materials store (XDMS, in development) and technical gas storage (XTGS, in development), I ventilation and air conditioning (XHVAC), J central workshop/stockroom (XHWS), K office building (XHO, in development), L visitor and conference centre, school labs (XHV, in development), M gate house (XHGATE)

Facility Development

With all the scientific instruments operational, 2020 was intended as the first year of full operation of the European XFEL. Unfortunately, due to the COVID-19 pandemic, experiments and facility development had to be significantly reduced. Nonetheless, some very important results were achieved.

This article highlights the status of projects underpinning the further development of the European XFEL facility. These development activities were carried out in addition to the operation programme. They included mechanical, software, and procedural work and often involved multiple groups from European XFEL and DESY.

Accelerator, FEL sources, and X-ray beam transport systems

The “Facility Development” beam delivery mode of the European XFEL made it possible to further develop the accelerator, FEL sources, and X-ray beam transport systems, with the strategic goal of increasing their overall performance and providing new features.

One focus in 2020 was the investigation of the electron beam trajectory in the undulator sections and systems. In order to improve the SASE performance, the beam trajectory of the electrons and photons inside the undulators must be extremely well aligned, and the strength of the magnetic field of the individual undulator segments (given by their so-called *K* value) must be well tuned. This was achieved by means of various electron- and photon-beam–based methods, building on the close collaboration of the XFEL group at DESY and the Undulator Systems, X-Ray Photon Diagnostics, and Controls groups at European XFEL. Studies were performed from the main control room, to which the signals from the X-ray devices had been routed.

Another focus was on studying the various elements affecting the stability of the X-ray beam, a major issue for the reliable operation of the scientific instruments. The X-ray beam position, the photon energy, the X-ray source location in the FELs, and the X-ray pulse arrival time fluctuate from pulse to pulse, and large deviations from the mean value lead to limitations in the stable and efficient operation of the scientific instruments. In addition, long-term drifts make the tune-up and optimization of beam parameters more difficult. To better understand and address these problems, a Stability Task Force was established in 2020, consisting of eight work packages, ranging from the systematic recording of environmental parameters, such as temperature and vibrations, to the optimization of diagnostic devices and software developments. Over 50 scientists and engineers from European XFEL and DESY cooperated in this task force, which is ongoing.

One of the first improvements was the implementation of an electronic cross hair on important imagers, allowing a precise and repeatable positioning of the X-ray beam in each FEL at the beginning of each shift. Accelerator controls for steering the electron beam by means of quadrupoles and correctors and for moving the pointing of the X-ray FEL beam were improved and optimized for stable operation. Another achievement was the use of high-speed cameras and the development of correlation analysis software tools, which now enable fluctuations of the X-ray beam position with respect to the electron beam monitors to be studied within one pulse train. Following this successful study, two permanent ports for such measurements are now being prepared in the X-ray beamlines. A third result was the reduction of the intra-train X-ray beam arrival jitter. For this purpose, the X-ray and electron beam arrivals were studied simultaneously at several scientific instruments and using electron beam arrival monitors. By careful implementation of feed-forward routines acting on the generation of the electron bunches, the arrival time jitter of the X-ray pulses at the scientific instruments could be reduced to 10 fs (RMS) during a pulse train. The next goals are to optimize the method and to make this performance available during regular user operation.

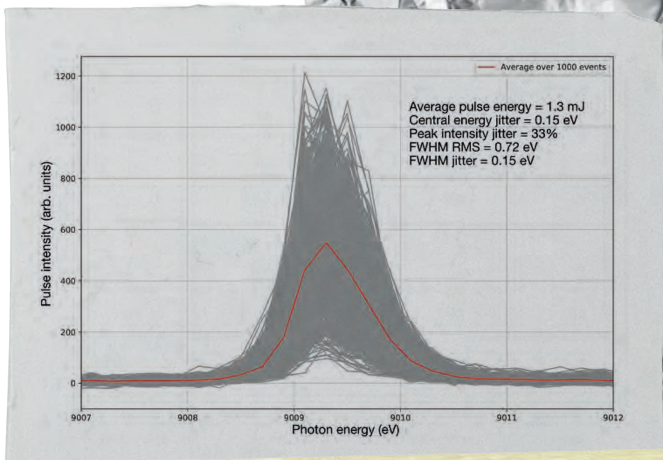


Figure 1: Spectra of HXRSS beam acquired with the HIREX spectrometer at SASE2. The average spectrum (red line, 1000 samples) is shown together with spectra from single X-ray pulses (grey lines).

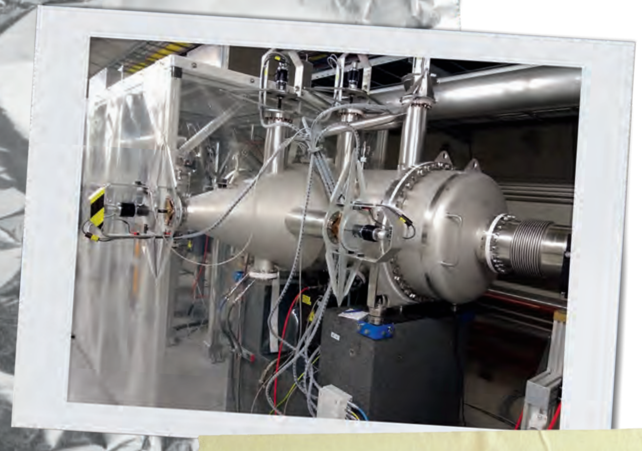


Figure 2: Vacuum chamber for the SXP distribution mirror during installation

A further area of activity was the study and development of new FEL delivery modes, potentially expanding the capabilities for scientific experiments at the European XFEL. This area benefitted significantly from the newly created FEL R&D group, which includes staff from the FEL Physics, Undulator Systems, and other groups at European XFEL as well as from the XFEL and Accelerator Physics groups at DESY. The successful implementation of an electron beam chicane at the SASE3 FEL for two-colour X-ray pump–probe experiments is highlighted in a separate article (see Technical Highlight). Another effort concerned the provision of hard X-ray self-seeding (HXRSS) at SASE2, a method for increasing the spectral brilliance of the X-ray light. Both methods will be available to experiments, and therefore to users, from 2021, albeit only in a special mode requiring close collaboration between experimenters and operators.

Self-seeding is based on the amplification of a narrow-bandwidth seed signal obtained by monochromatizing an initial SASE X-ray pulse [1]. Since the second half of 2019, a cascade of two transmissive diamond crystal monochromators has been available for this purpose at SASE2. In 2020, following undulator alignment efforts, HXRSS was demonstrated for both monochromators alone, as well as using them simultaneously, a mode envisaged to allow HXRSS operation at the European XFEL at high repetition rates. Self-seeded lasing was observed at different photon energies ranging from 9 keV to 13 keV. The highest spectral flux was obtained at a nominal photon energy of 9 keV, with an average pulse energy of about 1300 µJ—of which 700 µJ can be attributed to the seeded fraction—and a bandwidth of around 0.7 eV (FWHM, Figure 1). Operation at high repetition rate with up to 400 electron bunches at a frequency of 1 MHz showed no noticeable heat-loading effects, both at 9 keV and at 13 keV. At 9 keV, the intensity along the X-ray pulse train was almost uniform. Special self-seeding modes were tested, such as seeding multiple X-ray energies within the SASE bandwidth or second-harmonic radiation at 18 keV, the latter in both non-linear harmonic generation and coherent harmonic generation modes. The HXRSS results are extremely encouraging, and studies will continue to reach the expected performance limits.

Yet another new development was initiated: A set of studies concerned the creation of shorter X-ray pulses either through operation at reduced electron charge combined with stronger compression of the electron bunches, or through the non-linear manipulation of the longitudinal phase space, which enables a smaller and shorter fraction of the electron bunch to lase.

A completely different activity concerned the preparations for the new Soft X-Ray Port (SXP) scientific instrument at SASE3, which will complement the SQS and SCS instruments. The dedicated, about 60 m long SXP beam transport system consists of a distribution mirror (Figure 2), an exit slit, including a camera system allowing spectral analysis of the SASE beam, two additional imagers, and a beam shutter. SXP employs the same SASE3 beam offset mirrors as the other two instruments and has access to the soft X-ray monochromator, the gas attenuator, and various SASE3 X-ray diagnostic devices. In 2020, most of the SXP beam transport system was installed through a joint effort of the Vacuum, X-Ray Optics, X-Ray Photon Diagnostics, and Mechanical Engineering groups. A remaining imager and the distribution mirror will be installed in 2021 in preparation for first beam to the SXP hutch in 2022. In parallel, by the end of 2020, the construction work for the SXP instrument in the experiment hall started under the supervision of the Project Management Office and the Technical Services group. Following the construction of new rack rooms and a control hutch, the installation of the technical infrastructure will be completed in early 2021, paving the way for the installation of the instrument components. Major contributions to the funding of the beam transport components were provided by the TR-XPES user consortium through the universities of Hamburg and Kiel in Germany, based on a BMBF Verbundforschung grant.

In June 2020, a paper titled "A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator" [2], which describes the start of the European XFEL X-ray FEL delivery, was published in *Nature Photonics*.

Detectors and data sciences

The year 2020 brought many unexpected new challenges related to remote working, due to the worldwide COVID-19 pandemic. The IT & Data Management (ITDM), Controls, and Data Analysis groups of European XFEL ensured the continuity of work by providing necessary equipment and software tools to enable a smooth transition to large-scale remote operation. Of particular importance were the efforts to enable remote scientific experiments for the restart of the facility in the summer. Originally, the infrastructure for experiments was designed on the assumption that experiments would be performed by users coming to the facility. In 2020, however, European XFEL users were spread around the world and had to be given secure remote access to be able to directly monitor their experiments. ITDM provided the required tools for direct audio and video communication between the users and the European XFEL staff working directly in the experiment hutch, allowed access to all relevant information related to the status of the experiment, and made it possible to monitor extremely fast data streams and analyse the collected data quickly and remotely. The Controls group supplied a user-accessible, read-only Karabo interface to the instrument control systems and an SMS-enabled notification service that acts on events within the Karabo ecosystem, facilitating remote operation for both staff and users. The Data Analysis group provided an adaption of online data analysis tools, leveraging the interfaces supplied by the Karabo control system and offering rapid feedback even for remote operation. All these developments needed to be prepared and provided in a relatively short time in an environment with frequently changing experiment groups. The fruits of these efforts can clearly be seen in the plot showing the rate of collected data over the last three years, where the data rates in the second half of 2020 are similar to those seen in 2019 (Figure 3).

A major achievement for the Detector Operations group was the installation of the HiBEF AGIPD 0.5 Mpx detector prototype (Figure 4), performed in a joint effort with DESY and other European XFEL groups. This detector features the new application-specific integrated circuit ASIC-1.2 and new readout electronics, including newly developed firmware. The prototype was installed and successfully commissioned in the now operational detector laboratory in the European XFEL headquarters building, allowing a full system test, including standard control software, data acquisition system, and timing system. Using the detector laboratory considerably eased access to the detector during the initial testing phase and accelerated its later integration in the HED instrument. In November, the detector was then commissioned with X-ray beam, using X-ray delivery at a repetition rate of up to 4 MHz. The beam tests allowed the joint team from DESY, European XFEL, and the HiBEF user consortium to verify the performance of the new ASIC and readout electronics, test the integration into the data and calibration pipeline, and apply the detector in a first X-ray diffraction experiment. A couple of small issues were identified that will be addressed in the near future, but the detector could be

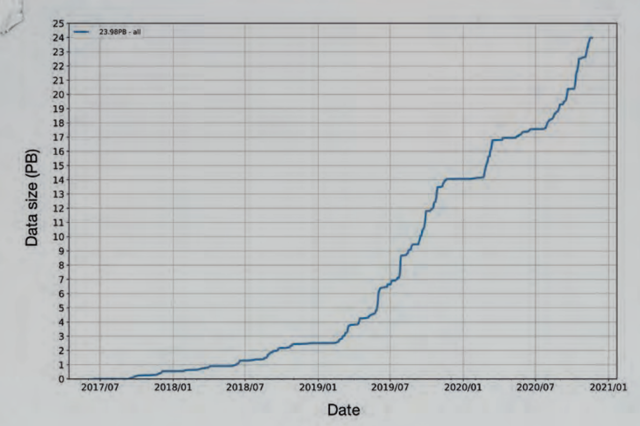


Figure 3: Time evolution of the raw data generated at the European XFEL scientific instruments

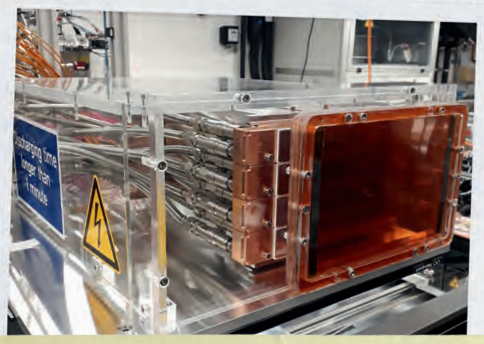


Figure 4: Mpx AGIPD detector tested in the detector laboratory and commissioned with X-ray beam at the HED instrument

used immediately to successfully collect high-repetition-rate data in a first experiment studying X-ray and laser heating of samples in diamond anvil cells. X-ray pulse-resolved diffraction using this new detector could be combined with a streaked optical pyrometry setup for time-resolved temperature measurements. This new platform at HED opens the way for qualitatively new science in diamond anvil cells in a series of high-pressure community proposals scheduled for 2021, for which this prototype detector will be employed.

A highlight from the Electronic and Electrical Engineering (EEE) group involved work on the conversion of fast and sensitive analogue signals from sources such as photodiodes, diamond detectors, and multichannel plates into digital samples, which is a crucial step in the data acquisition chain. Because of the high repetition rate of the European XFEL and the desired high resolution of the measurements, both the sampling rate and the so-called vertical resolution (e.g. the number of bits per converted sample) have to be pushed to the highest possible level—which is limited by current technology. In 2020, the latest generation of high-speed digitizers from Teledyne SP Devices—ADQ7 and ADQ14—were integrated into the European XFEL MicroTCA-based electronics (Figure 5). For this purpose, the EEE group developed, integrated, and verified firmware for the built-in field-programmable gate array (FPGA), which is required to allow accurate synchronization and preprocessing of the acquired signals before transferring the data with high-speed interconnects to the control system software Karabo. The Controls group developed the corresponding software and integration into Karabo to allow the operation of the card and the visualization, processing, and analysis of the acquired data.

Another major activity for the Controls group in 2020 was the introduction of the InfluxDB time series database. In August, Controls and ITDM jointly rolled out the system, which replaces proprietary text-based logging of the hundreds of gigabytes of archival data that the Karabo control system of the European XFEL produces annually. InfluxDB is used and developed by a large community and allows for rapid access to historic data, as well as highly configurable visualization and investigation thereof, using state-of-the-art solutions such as Grafana (Figure 6).

In 2020, the Data Analysis group focused on online data analysis, which is required to give experimenters faster and more detailed insight into their data at the moment it is recorded. A new collection of tools collectively called EXtra-metro was developed and introduced at the first scientific instruments. Being easily reprogrammable *in situ*, it can be adapted quickly to any experiment. This tool offers the possibility to perform specific calculations and

Figure 5: MicroTCA card for high-speed digitizers

Figure 6: Grafana panel showing InfluxDB-provided data on the status and messaging rates from the SASE3 programmable logic controllers for the previous seven days

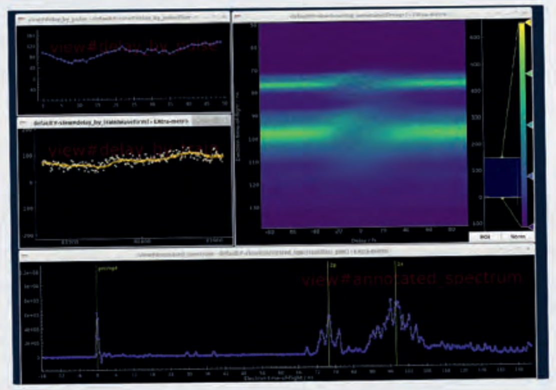


Figure 7: Live analysis panel visualizing pump–probe delay-dependent electron spectra at the SQS instrument using the high-performance client EXtra-metro

display their results online (Figure 7). This development built on improvements to the existing online analysis solution EXtra-foam and involved a significant effort on the part of all groups in the Data Department to ensure stable operation of the online calibration pipeline for the large photon detectors AGIPD, LPD, and DSSC.

Scientific instruments

In a collaborative effort between the Data Analysis group, the SPB/SFX instrument group, and experts from the group of Henry Chapman at DESY, a largely streamlined pipeline for analysis of European XFEL serial crystallography data was developed in 2020. The prototype pipeline called XWiz accepts data collected using the MHz-rate AGIPD detector or the JUNGFRAU detector at the SPB/SFX instrument and processes these, yielding the reduced data that synchrotron-experienced crystallographers are accustomed to. The workflow—currently relying on the CrystFEL software suite—takes data from the European XFEL calibration pipeline, identifies sample “hits” with Bragg diffraction peaks, and evaluates those individual detector frames with “hits” such that a list of unique crystallographic intensities is derived from the two-dimensional diffraction patterns (Figure 8). The data emerging from the pipeline can be further analysed using standard crystallography software tools and thus enables crystallographers to analyse serial crystallography data collected at the European XFEL without special expertise. At the end of 2020, the WZiz pipeline was in an advanced test phase with SPB/SFX scientists. It is planned to be rolled out for tests with beamtime users and near-live data in 2021.

In 2020, with strict travel restrictions, remote sample handling turned into a key feature towards establishing serial femtosecond crystallography (SFX) at X-ray FELs as a standard procedure for structural biology. The Sample Environment and Characterization (SEC) group succeeded in providing a workflow for remote sample handling. As part of this workflow, the XBI labs, funded by the XBI user consortium, provided the equipment and facilities for on-site crystallization and quality control of the samples; filling of sample reservoirs was performed by the XBI labs staff; and in order to ensure problem-free jetting of the crystal suspensions, SEC liquid-jet experts were present in every shift of a user experiment. With the additional possibility of testing samples prior to injection at the instrument under real-live conditions, European XFEL was able to offer an SFX sample handling workflow that supports the remote execution of user experiments.

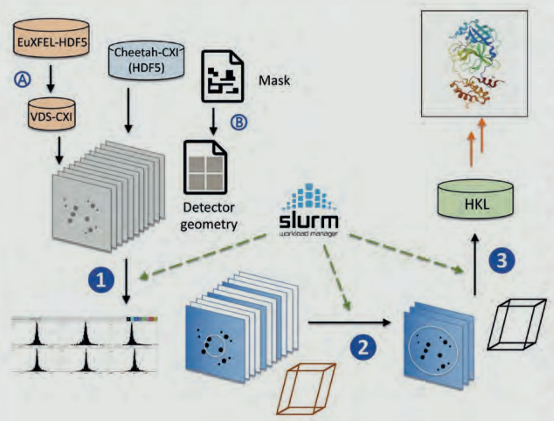


Figure 8: Schematics of the XWiz pipeline for SFX-type experiments, including peak finding and unit cell determination (1), selection of indexable images (“crystal hit frames”) and unit cell refinement (2), and identification of indexable images and unit cell refinement (3). Crystallographic scaling and intensity averaging yield a unique reflection data set.

The installation and commissioning of an X-ray gas monitor detector (XGMD) for pulse-resolved measurement of the X-ray pulse energy at the sample location was a major advance at the FXE instrument. The knowledge of pulse energies is important not only for the experiments but also for the optimization of the beam transport, where losses occur in the mirror reflections and the refractive optics. Furthermore, absolute pulse energies are needed for example to investigate material damage. The XGMD is optimized to measure the incident X-ray power of an FEL beam with absolute calibration. This measurement of power, together with the known effective repetition rate of the X-ray pulses, allows the average pulse energy to be calculated. In 2020, the XGMD in the downstream region of the FXE hutch was put into operation in a joint effort by the FXE, X-Ray Photon Diagnostics, EEE, and Controls groups. When the experimental geometry permits, the device is now routinely used for beam alignment and monitoring of the X-ray pulse energies. The XGMD also provides a measure of individual X-ray pulse energies, albeit only on a relative scale. The correlation of the single-pulse values with data provided by another intensity monitor of FXE shows very good linearity and confirms the concept (Figure 9). The optimization and integration of the XGMD data into the data acquisition will be a task for 2021.

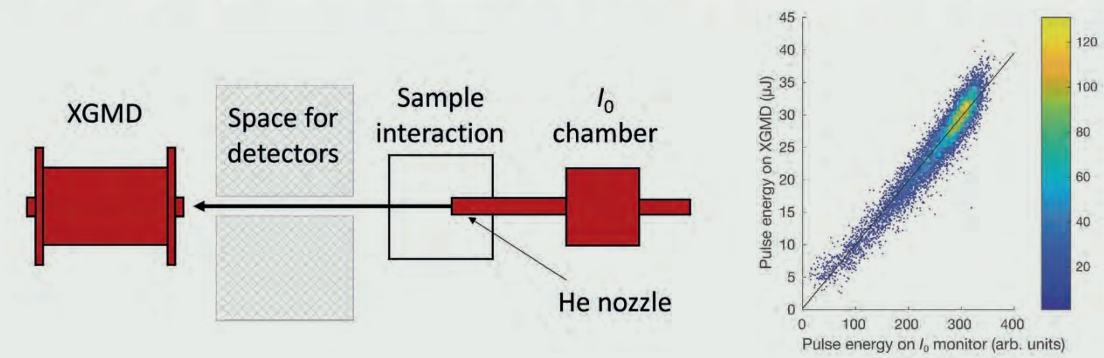


Figure 9: Schematic of the beam path through the FXE instrument. The beam passes first through a chamber measuring the incident intensity I_0, interacts with the sample (cylindrical liquid jet, not shown), and is then detected further downstream by the XGMD. The plot shows the correlation between both pulse energy monitors, with the pulse energy on the XGMD not corrected for air transmission (15%).

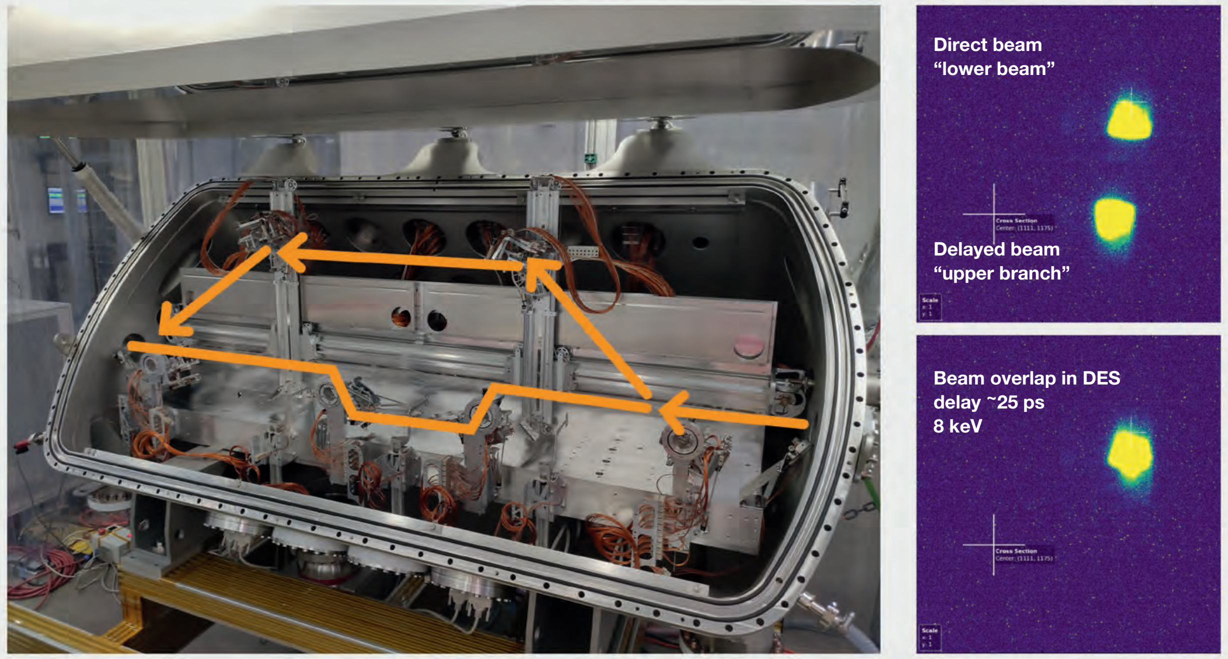


Figure 10: Left: MID SDL device inside the open vacuum chamber with the mechanics and optics visible inside. The orange arrows indicate the X-ray beam paths with the upper and lower branch. Right: Images of the two emerging 8 keV X-ray beams at the MID diagnostics station show the split beams (top) and spatial overlap (bottom) after tweaking the SDL mechanics (beam merger). In one of the beams, the X-ray pulses are delayed by 25 ps versus those in the other beam.

The X-ray split-and-delay line (SDL) at the MID instrument was installed in the ultrahigh-vacuum section of the instrument (optics hutch) during the winter of 2019–2020. The crystal-based MID SDL targets operation between 7 and 10 keV and delay times up to ~800 ps. The SDL divides the X-ray beam in two by means of a split crystal, and the split beams propagate in two separate optical branches with an adjustable path length difference, thereby creating a time difference between the pulses (Figure 10). A beam merger optics allows the pulses from the two branches to be recombined and spatial overlap to be achieved at the sample. Due to the restrictions caused by the pandemic, the commissioning of most of the functionalities of its high-precision mechanics could be achieved only in August and October 2020. Initial operation of the SDL at photon energies of 8 and 9 keV could be successfully demonstrated, and commissioning will continue in 2021 to progress towards unique dynamics and imaging experiments. The device was developed in collaboration with TU Berlin and the Max Born Institute (MBI) in Berlin, Germany, based on two BMBF Verbundforschung grants.

At the HED instrument, great progress could be achieved in the integration and use of the various optical laser sources. The performance and integration of the ReLaX optical laser at the 100 TW level (3 J, 30 fs—already commissioned as a stand-alone system at the end of 2019) were successfully demonstrated in combination with the X-ray beam. The temporal arrival jitter with respect to the X-ray pulses was measured to be less than 30 fs (RMS) at the sample location. To be used with this laser, a platform for small-angle X-ray scattering (SAXS) [3] was successfully commissioned. It consists of a cylindrically bent highly annealed pyrolytic graphite crystal deflecting the SAXS signal to the X-ray detector and

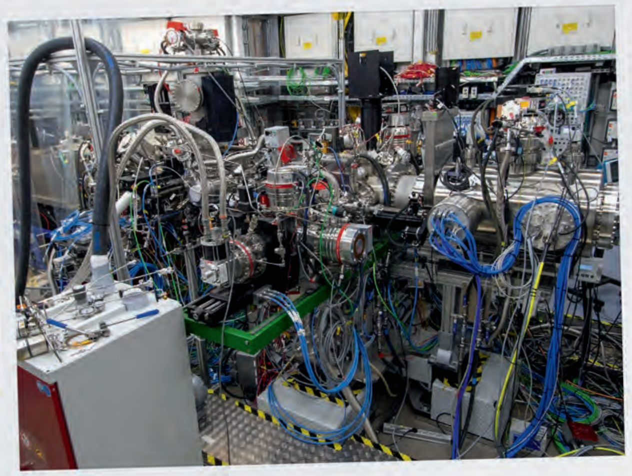


Figure 11: SQS hutch with the KB optics and the two interaction zones AQS and NQS

thereby reducing the strong bremsstrahlung background originating from the laser-induced plasma formation at the sample. The second large laser system DiPOLE 100-X was delivered at the end of 2019 from the Central Laser Facility in the UK and installed, and commissioning started. First light at the sample location is planned for the second half of 2021. In addition, in 2020, a first user experiment was performed using the pump–probe (PP) laser with 400 nm frequency-doubled pulses. The surface structure modification on 50 nm thick gold following laser irradiation was investigated by means of grazing-incidence X-ray scattering. The temporal jitter between the PP laser and the X-ray beam was optimized to be shorter than 30 fs (RMS), measured by the photon arrival monitor (PAM) permanently installed at HED 10 m upstream of the sample position. The HED PAM is quasi non-invasive, with only a few percent of X-rays being absorbed.

An essential step to further improve the performance of the SQS instrument was realized in 2020 with the installation and commissioning of the new focusing optics for the soft X-ray beam. Two highly polished, 80 cm long, bendable Kirkpatrick–Baez (KB) mirrors have replaced the former mirrors of fixed radii, which served as an interim solution. The bendable KB mirrors provide much more flexibility for experiments by enabling control of the focus size in the interaction region and of the focus position along the beam propagation direction. This latter option is particularly important because it provides the possibility to install two experiment stations in series, thereby completing the initial design concept for the SQS instrument. In this way, the time and workload needed to exchange the different experiment chambers—AQS, NQS, and REMI—is drastically reduced. Changing between experiments is now possible within minutes through the adjustment of the KB mirrors and does not require removal and reinstallation of an entire experiment station as before (Figure 11). Installation, alignment, and first commissioning of the KB mirrors were performed in a collaboration between the SQS and X-Ray Optics groups using a Hartmann-type wavefront sensor, provided by the FLASH Photon Beamlines and Optics group at DESY and LaserLab Göttingen, as well as conventional time-of-flight ion spectroscopy available in all experiment chambers of SQS. The first measurements confirmed the results of simulations for the optics, which predicted a small focus of 1–1.5 μm diameter and a slightly larger focus of 2–3 μm diameter in the first (F1 and F1') and second (F2) focus position, respectively. These focusing conditions allow intensities of a few 10^{18} W/cm^2 to be created in the interaction regions, which are ideal preconditions for all investigations of non-linear phenomena at the SQS instrument.

X-ray absorption spectroscopy (XAS) has been successfully established at the SCS instrument. XAS is a widely used technique to study local structure and oxidation states of atoms in solids and molecules on surfaces or in liquids, and FELs promise to add femtosecond time resolution. Its implementation at FELs is challenged by the required high spectral sensitivity, while having to overcome very high shot-to-shot intensity fluctuations when employing monochromatized SASE radiation. The SCS group has adapted a scheme developed at LCLS in the USA using diffractive optics to create copies of the incoming beam [4]. The SCS implementation uses a transmission grating, provided by the group of Christian David at the Paul Scherrer Institute (PSI) in Switzerland, producing three beams of equal intensity (0th, +1st, and -1st diffraction order) propagating onto a single module of the DSSC detector in three well-separated areas. Each beam illuminates many pixels to achieve a high signal-to-noise ratio. Two identical samples and a reference substrate are placed in the three beams slightly after the

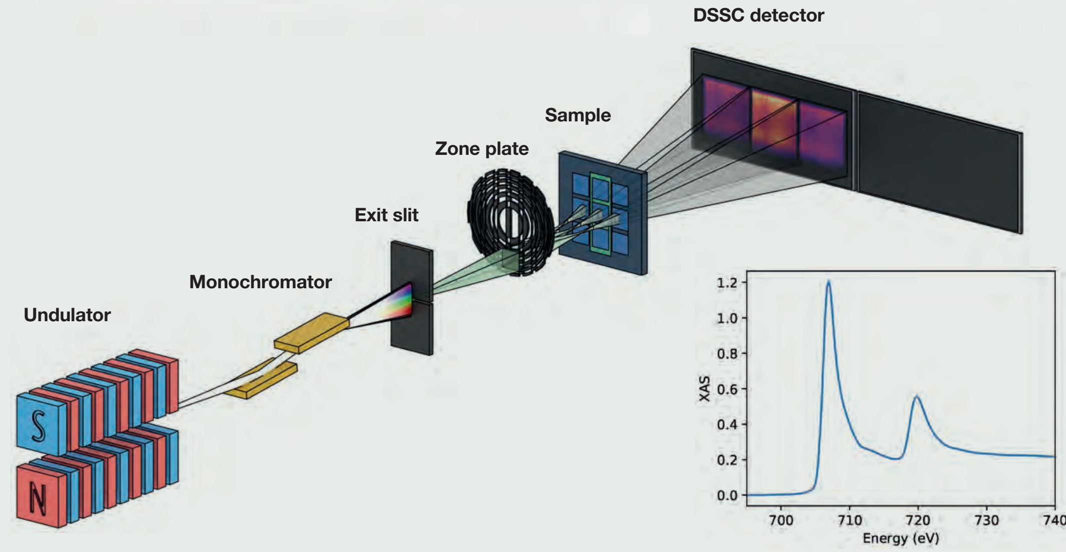


Figure 12: Schematic showing the collection of XAS spectra (example for Fe $L_{3,2}$ edges) at the SCS instrument by scanning the SASE3 undulator gap and the soft X-ray monochromator. An off-axis zone plate splits the monochromatized X-rays in three beams of equal intensity and focuses them onto sample and reference membranes. The normalized intensities are probed by integrating the pixel counts from the DSSC detector.

zone plate focus, allowing ground-state, excited-state, and time-resolved XAS signals to be determined (Figure 12). To record XAS spectra, the monochromator is scanned continuously back and forth between two energy end points with the help of a middle layer device developed by the Controls and X-Ray Optics groups. The undulator gap follows the monochromator scanning in order to match photon energies using a communication protocol developed by the Controls, X-Ray Optics, and Undulator Systems groups. Two community proposals were dedicated to the commissioning of this scheme. The first, led by Martin Beye (DESY), studied non-linear XAS taking advantage of the high X-ray fluence at the zone plate focus. The second, led by Andrea Eschelohr (University of Duisburg-Essen), performed first femtosecond pump–probe experiments. The DSSC detector allows up to 680 X-ray pulses to be recorded per pulse train, but so far XAS experiments had to be restricted to around 20 X-ray pulses per train due to the limited heat dissipation in the investigated solids. For even more sensitive samples, the sensitivity of the XAS platform at SCS even allows measurements with a single X-ray pulse per train at 10 Hz, employing the fast sample scanner system developed by the Sample Environment and Characterization group (Carsten Deiter).

References

[1] G. Geloni, V. Kocharyan, E. Saldin: “A novel self-seeding scheme for hard X-ray FELs”, J. Mod. Opt. **58**, 1391 (2011), doi:10.1080/09500340.2011.586473;
S. Liu et al.: “Preparing for high-repetition rate hard X-ray self-seeding at the European X-ray Free Electron Laser: Challenges and opportunities”, Phys. Rev. Accel. Beams **22**, 060704 (2019), doi:10.1103/PhysRevAccelBeams.22.060704

[2] W. Decking et al.: “A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator”, Nat. Photonics **14**, 391 (2020), doi:10.1038/s41566-020-0607-z

[3] M. Šmíd et al.: “Mirror to measure small angle X-ray scattering signal in high energy density experiments”, Rev. Sci. Instrum. **91**, 123501 (2020), doi:10.1063/5.0021691

[4] W. Schlotter et al.: “Balanced detection in femtosecond X-ray absorption spectroscopy to reach the ultimate sensitivity limit”, arXiv:2006.1396 (2020)

Company Development

As in other research facilities, the impact of the COVID-19 pandemic on the general development and related administrative processes has been significant.

In order to protect staff members and users as well as the large capital investment for the accelerator and other instumentation against possibly severe damages in case of an uncontrolled curfew-related complete shutdown, the European XFEL Management had to take far-reaching decisions, like ending User Run 5 early, postponing the remaining experiments to the fall of 2020, and postponing User Run 6 to the beamtime scheduled in spring 2021. This also required shifting the 7th call for proposals from June to autumn 2020. In addition, the facility went into a reduced mode of operation, with minimal staff on site and extended use of home office.

During 2020, the regulations put in place by the local authorities and the German government, were strictly followed, and no case of infection of an employee was reported.

Hygiene measures were implemented, with handwashing guidelines in all restrooms and kitchens, disinfectant supplies in the hutches, increased cleaning of buildings and infrastructure, and additional safety measures taken in the company restaurant, BeamStop. A regular task force meeting was set up with the Managing Directors and representatives from relevant administrative and operational groups to discuss, implement and adapt appropriate measures for the different phases of the pandemic.

The planning with uncertain boundary conditions was challenging. Administration was one of the key areas where personnel needed to be onsite to perform their work. For instance, tasks like contract management, salary transfers, hiring, bank business, and procurement had to continue without any delay during the lockdown and reduced operation.

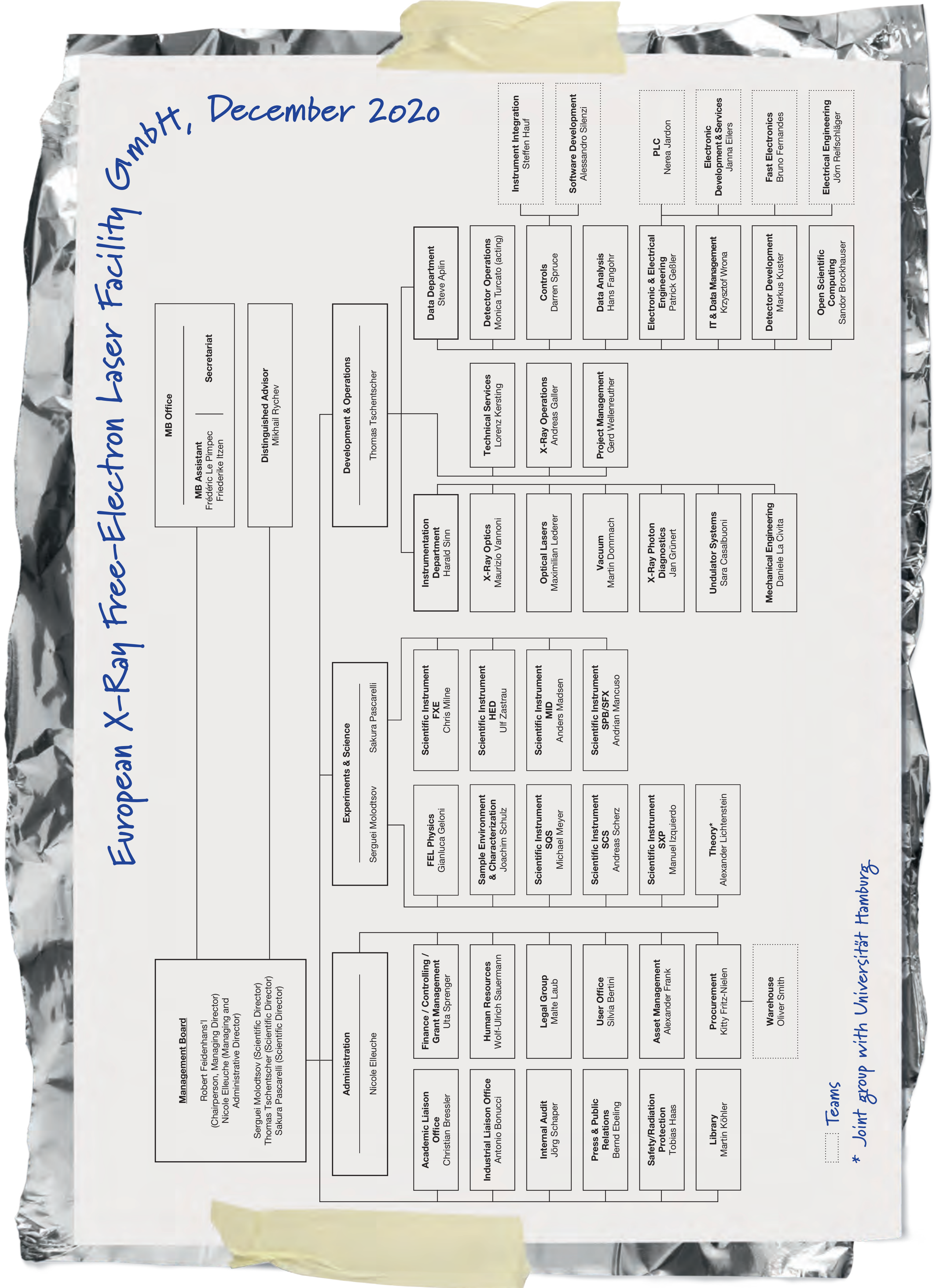
Consequently, to secure safe working conditions for the staff members who were required to be onsite, the maximum occupancy of all rooms was defined and distancing rules were strictly maintained. Offices could be used by only one person at a time. For tasks that did not allow maintaining a distance of 1.5–2 m between staff members, protective equipment was provided by the company.

To reduce the pressure on families when kindergartens and schools were closed, the company, on request, awarded up to 20 extra days of childcare to support staff with children.

The working situation during the pandemic has shown that there is an opportunity for organizations to rethink the way employees work and collaborate, also remotely, to increase the organizational agility and be more competitive in a complex and dynamic environment. For example, a new works agreement on remote work was negotiated to set the framework for working from home, or even other places, if agreed with the company. The European XFEL procedures for signatures were adjusted to reduce manual signatures to a minimum and allow other options, such as scanned signatures or approvals by email for internal processes where applicable.

The effect of the listed measures on the development of the annual operation budget of European XFEL is still challenging to estimate. A comparison with the cost development in 2019 provides insights on the financial impact caused by the pandemic. It assumes that standard operation years follow—on average—similar spending patterns and forecasts the 2020 budget, including planned budget increases in some areas. In summary, reduced spending until the end of the year is expected for electricity, purchases, and travel/accommodation. On the other hand, in the areas of IT / technical infrastructure and personnel, the expenses are projected to be higher than originally calculated. For example, the number of purchase orders and the total value of expenses decreased by 20% as compared to 2019. However, the decrease in recurrent costs is partly balanced by increasing expenses on personnel due to delays in construction or commission work or because specific projects have to be extended, for example, projects for postdocs and Ph.D. students. The general principle of the company is to not create disadvantages for European XFEL. This could happen if non-permanent staff members would have left without finalizing their corresponding work, which was avoided by extending their contracts. The extraordinary extension of a number of contracts might have a long-term effect, which we will have to scrutinize in more detail before we can report on general savings or increased costs due to the pandemic.

Organizational changes like reporting structures, workflows and meeting organisation were implemented during 2020, and an increased use of digital tools for different processes is planned for 2021. In particular, the start of the new Enterprise Resource Planning (ERP) Program will be a milestone for the modernization of administrative processes.



Budget and Third-Party Funding

At the end of 2020, 98.5% of the European XFEL construction budget was spent. The annual operation budget was 132 million euro (M€) in 2020 and is going to increase to 133 M€ in 2021.

Budget
Parallel to the operation budget, the investments of the remaining construction budget continued for the remaining buildings. The management of fixed assets was improved, and the reorganization process was supported by the Controlling group.

The **overall construction budget** of the European XFEL amounts to around 1.25 billion euro (2005 value). Forty-six percent of the project volume was contributed in kind by various partners. The remaining fraction of more than 650 M€ (2005 value) was contributed in cash to the company by its shareholders and associated partners.

At the end of 2020, 98.5% of the total cash budget for construction was spent. The **total European XFEL operation payment budget** in 2020 amounted to 132.5 M€, and the amounts for the finalization of the construction phase were approved in the previous year and therefore transferred to 2020.

The major activity in operation “beamlines and experiments” had a total budget of 52.8 M€ (40.0%); certain activities were prioritized to reach their goals in 2020. For “machine and technical infrastructure”, with a total budget of 59.9 M€ (45%), 57.1 M€ was spent on the operation of the accelerator.

Personnel costs including staff from DESY were the largest part of the costs, with 44% and 58.6 M€, and increased in 2020 due to the reduced construction activities. A smaller portion of 52.6 M€ was spent for recurrent personnel.

For 2021, an increased annual payment operation budget of 137.3 M€ was approved by the European XFEL Council.

Besides the core funding by the shareholder countries, third-party funding plays an increasing role within the budget portfolio of European XFEL, providing flexibility for important projects. The European Union, within the framework of its Horizon 2020 research and innovation programme, and the German Research Foundation (DFG) are examples of the types of prestigious funding bodies making these contributions, underlining the high quality of research projects performed by European XFEL scientists.

Third-party funding
In 2020, European XFEL participated in 12 research projects, seven of which were funded by Horizon 2020 and Interreg, and five by national funding organizations such as DFG and the German Federal Ministry of Education and Research (BMBF).

The overall income of these projects was 4.4 M€, of which 75% came from European funding and 25% from national funding. The funds spent by third-party projects amounted to about 1.4 M€ in 2018, 0.9 M€ in 2019, and 1.1 M€ in 2020.

In 2020, 10 staff members were employed exclusively for third-party-funded projects. Three projects ended in 2020, and two new projects were started.

Call for R&D projects
In spring 2020, European XFEL issued its second call for photon-based research and development (R&D) proposals, open only to staff members of European XFEL and DESY.

To fulfil the short-term strategic goals of European XFEL, focused on completing the instruments, and to reach these goals with respect to automation of data collection and analysis, the management board decided to assign R&D funds of the call 2020 to three categories of projects. In addition, a separate topic was included, anticipating the situation of the pandemic with the intention to provide funds for urgently needed support activities on short notice.

1. Data issues
2. Instrument completion
3. “Blue sky” research
4. Covid-19–related user support

Thirty applications were received, covering a broad range of topics and being well distributed over the four different categories (see Fig. 3).

Total budget 2020

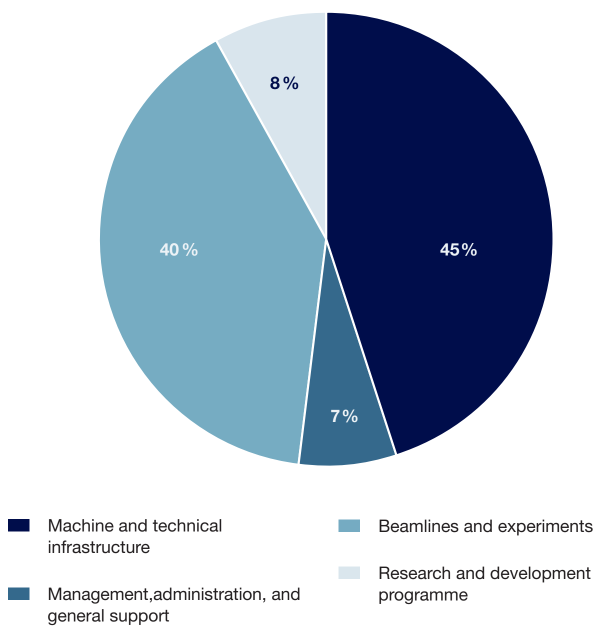


Figure 1: Payments by major activity in 2020

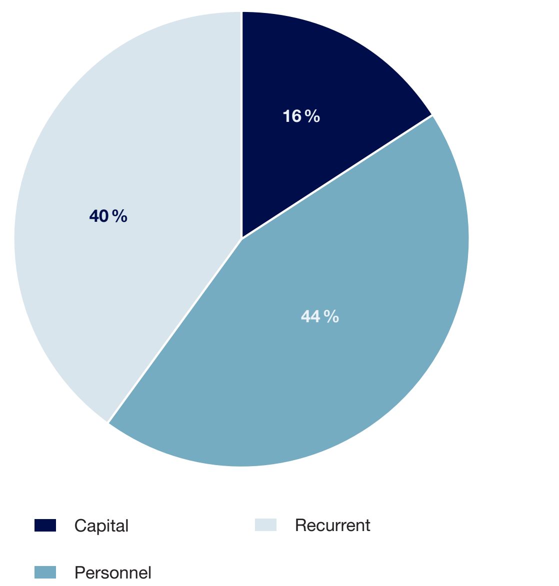


Figure 2: Payments by budget items in 2020

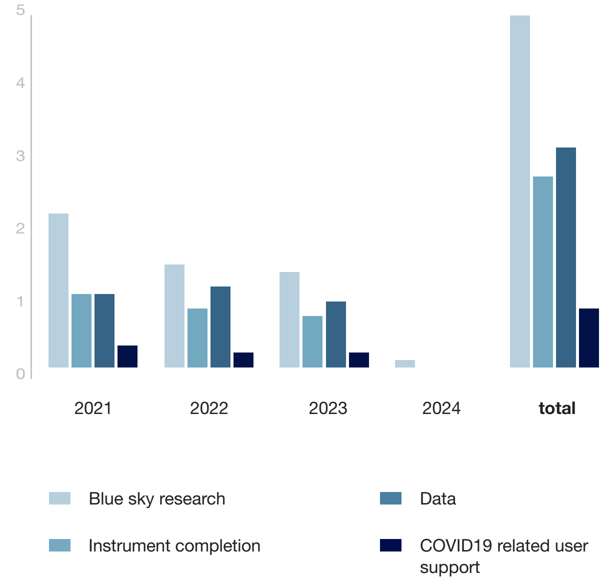


Figure 3: Overview fund distribution for projects in the area of R&D

Table 1: Overview of calls for R&D funds (2019–2020)

	2019	2020
Deadline	May 2019	May 2020
Selection	July 2019	July 2020
Allocation	September 2019	July 2020
# submitted proposals	32	30
# approved proposals	11	28
Allocated Budget	4.4 M€ over 3 yrs	11.2 M€ over 3 yrs
Allocated FTE	11-15 FTE/yr	25-28 FTE/yr

A total of 24.5 M€ in funding was requested, far more than could be granted. Twenty-eight proposals have been awarded funding but were partially adjusted in terms of funding or scientific scope. Each of the projects will run for a maximum of three years and have an annual budget of up to 300 thousand euro (k€). They will start in 2020 with funding of 3.5 M€ for the first year. The total budget for all the projects within the three years amounts to 11.2 M€.

Quality Management in Safety and Administration

Quality management (QM) at European XFEL comprises different quality-oriented services, procedures, and guidelines. The intent is to blend international quality management of scientific institutions and research infrastructures with the latest thinking on the administration of bigger service units with special regard to safety and reliability requirements.

The focus of the activities established and procedures implemented or adapted during 2020 was a different quality opportunity: meeting the needs of European XFEL users, improving processes, involving staff members and partners in quality improvement, and ensuring sustainable and reliable facility operation. In particular, the reporting requirements of European XFEL shareholder countries as well as the legal boundary conditions for administrative processes were addressed.

Particular focal points are safety and radiation protection, implementation of an enterprise resource planning (ERP) system, and further development of risk management and assessment. Besides these activities, regular internal audits as well as an external end-of-year audit are part of our QM strategy, and the results were reported to the management board.

Safety and Radiation Protection

Activities during 2020 were strongly affected by the COVID-19 pandemic. From the second quarter, the presence of employees on the European XFEL site was strongly reduced, with many staff members working from home office. This is reflected in the accident statistics shown in Table 1.

2020	Minor accidents	Declared accidents	Commuting accidents	Total
Q1	10	5	8	15
Q2	3	1	1	4
Q3	4	0	2	4
Q4	6	1	2	7

Table 1: Number of work accidents during 2020 for each quarter. Declared accidents are those resulting in an absence of more than three working days. All other accidents are considered minor accidents. Commuting accidents may be minor or declared accidents.

Many employees used the time in home office to work on documentation projects, such as risk assessments. Significant strides were made to complete the risk assessment documentation related to all aspects of work at European XFEL.

The pandemic also generated a push to increase the role of e-learning in the area of safety training. A complete revamping of the online safety training system for European XFEL was initiated. The new system will be tailored to the specific needs of European XFEL and will seamlessly integrate the safety training requirements of users, guests, contractors, and employees. It will also interface directly with the access control management system and thus save significant effort currently needed to keep access permissions and training requirements up to date.

Finally, the so called “Active Instrument Beamstop” project was initiated and completed. Active Instrument Beam Stop is part of the beam containment system and is placed at the end of the experimental stations. It stops the delivery of XFEL beam to the experimental stations if it detects the XFEL beam. This additional safety layer will allow to lift operational restrictions that are currently needed for radiation protection.

Risk Management

In 2020, European XFEL management decided to update the Risk Register tool, which was initially based on a spreadsheet file. Following our risk guidelines and due diligence, a project was launched to move our risk register to a cloud-based database that provides more data security and reliability. Its deployment is scheduled for February 2021.

International Collaboration

European XFEL maintains an extensive international research network with partners around the world. In 2020, existing and new collaborations helped to further advance X-ray science and the unique research opportunities at the facility.

Within the European Framework Programme Horizon 2020, European XFEL collaborates in the following projects:

- ATTRACT (GA No. 777222)
  Breakthrough Innovation Programme for a Pan-European Detection and Imaging Ecosystem
- CALIPSOplus (GA No. 730872)
  Convenient Access to Light Sources Open to Innovation, Science and to the World
- CREMLINplus (GA No. 871072)
  Connecting Russian and European Measures for Large-scale Research Infrastructures
- EDAX (GA No. 669531)
  Beating Complexity through Selectivity: Excited state Dynamics from Anti-Stokes and non-linear resonant inelastic X-ray scattering
- MS SPIDOC (GA No. 801406)
  Mass Spectrometry for Single Particle Imaging of Dipole Oriented protein Complexes
- PaNOSC (GA No. 823852)
  Photon and Neutron Open Science Cloud

Together with Lund University in Sweden and TU Berlin in Germany, European XFEL participates in the InVision project within the Röntgen-Ångström Cluster (RÅC), a Swedish–German research collaboration in the fields of materials science and structural biology that aims to strengthen research at synchrotron and neutron radiation sources. InVision is dedicated to improving the understanding of the dynamics of metallic foams and granular matter using sub-microsecond single-shot multiprotection X-ray imaging.

European XFEL is part of the Hanseatic League of Science (HALOS), a project fostered within the European Regional Development Fund Interreg Öresund-Kattegatt-Skagerak (ÖKS) programme. HALOS builds a unique collaboration between Hamburg and southwest Scandinavia, bringing together four unique research facilities—MAX IV, ESS, DESY, and European XFEL—and creating a centre for integrated, world-leading life science innovation and research.

The League of European Accelerator-based Photon Sources (LEAPS) strengthened its cooperation on finding new pathways into the post-corona era by making the LEAPS research infrastructures more resilient towards pandemic crisis situations, supporting European society in the fight against infection and the development of a circular economy within the scope of the European Green Deal and Missions of Horizon Europe (Digital LEAPS).

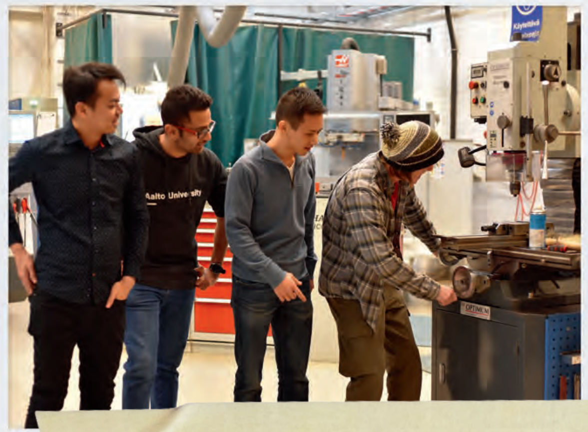


Figure 1: M.Sc. students have been working on prototyping social innovation solutions inspired by ATTRACT projects. ATTRACT organized a workshop in January at Aalto Design Factory where the students shared their experience and brainstormed about future steps.

In July 2020, European XFEL, together with DESY, published the summary report of the International FEL Expert Meeting on the potential dual use of free-electron lasers, held in November 2019. The report, titled "Use of free-electron lasers and beyond: Scientific, technological, and legal aspects of dual use in international scientific cooperation", is available in the European XFEL publication database [1]. The aim of European XFEL and DESY is to see this report disseminated widely to other research infrastructure in order to raise awareness among scientific institutions.

At the end of the year 2020, activities imbedded in the International Laboratory on Free-Electron Laser Science and Technology were resumed after 20 months of pause, thanks in part to the results published in the above-mentioned report. The lab—created jointly by the Chinese Academy of Science and the Helmholtz Association, and led by DESY in Germany and by SARI in China—has a budget of 1.2 million euro per year for five years. European XFEL participates in the development of new photon sources and in other scientific fields of research, like fast processes in chemistry or in structural biology.

Figure 2: CREMLINplus kick-off meeting at DESY on 19 February 2020

Within the Baltic Science Network initiative, European XFEL experts strongly supported the overall initiative led by the Hamburg's Ministry of Science and Research (Behörde für Wissenschaft und Forschung, BWF), notably by organizing a meeting notably by organizing a meeting to support the launch of a student (BSc and MSc) mobility programme BARI [2] in Hamburg. The second activity involved the strengthening of scientific collaboration around the Baltic Sea region in academia but also with industry [3].

The Launchpad symposium was held virtually in Riga, and European XFEL provided, beyond the organization committee, a scientific oral presentation and contributed to two proposals in collaboration with Russia and the HALOS project. All collaborative proposals submitted are under evaluation, and results will be known in early 2021.

[1] https://xfel.tind.io/record/2268
[2] https://www.baltic-science.org/bari/
[3] https://www.baltic-science.org/launchpad-3steps/

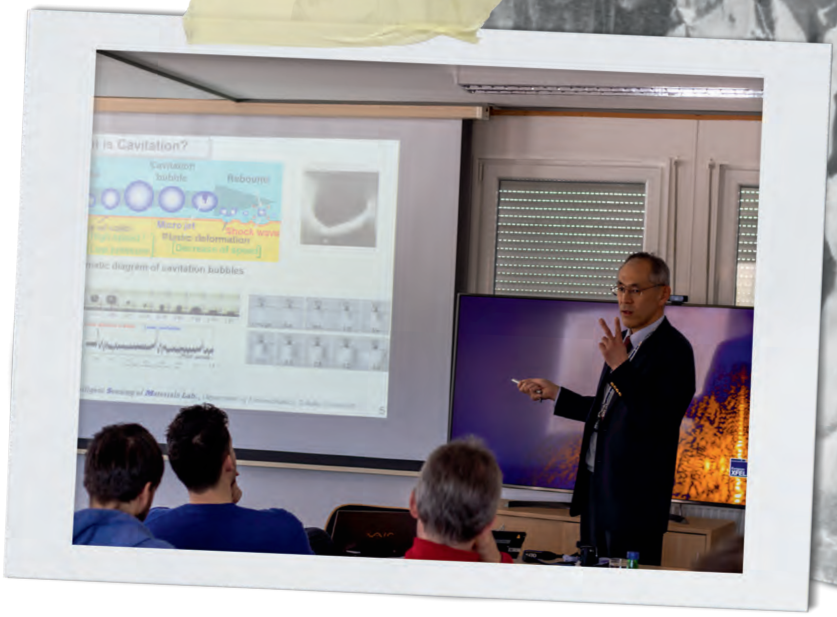


Figure 1: Hitoshi Soyama of Tohoku University, Japan, gave a presentation on cavitation peening and its industrial applications in early March 2020.

Contacts to Industry

In 2020, the main achievement of the European XFEL Industrial Liaison Office (ILO) was to kindle the interest of companies and applied-science research institutes in using the European XFEL facility for industry-related applied science.

In particular, representatives of Airbus and the ZAL Centre for Applied Aviation Research met expert scientists from European XFEL to better understand how the company could contribute to their development programme. One possible application could be laser shock peening, a process in which a laser beam is focused on the surface of a metal in short patterned pulses in order to improve the stress profile of the bulk to prevent cracking due to metal fatigue and failure. Some preliminary exchange was conducted to understand at which level an X-ray FEL can contribute to the basic understanding of the process.

“To have such a facility near the Airbus centre is a great opportunity for collaboration that can promote the innovation excellence in the Hamburg area,” says Domenico Furfari of Airframe Research & Technology at Airbus Operations. “It is motivating to see that the instrumentation we have built primarily for fundamental research at extreme pressures and temperatures shows a very promising potential also for advancing high-level industrial research,” says Ulf Zastrau, who is responsible for the HED instrument at the European XFEL. “We look forward to discussing how laser peening can be optimized in collaboration with Airbus and ZAL.”

A very interesting connection was established with Alexander Korsunsky, a professor at the Rolls-Royce University Technology Centre in Solid Mechanics at the University of Oxford, UK, and Hitoshi Soyama, a professor in the Department of Finemechanics at Tohoku University in Japan. Alexander Korsunsky is an expert in processing–stress–performance relationships for aerospace component design and a world-leading proponent of synchrotron, neutron, electron, and ion beam methods for microscopy and stress analysis. Hitoshi Soyama is developing novel peening methods and apparatuses. The key topic of the growing collaboration of European XFEL with these two professors is wet cavitation peening, which opens up unprecedented opportunities for the surface treatment of aviation engine components as well as in the biomedical field.

“The MHz frequency of tomography acquisition will allow first time-resolved observation of cavitation phenomena to understand the physical mechanisms, predict consequences for material structure and deformation, and optimize processing to ensure structural integrity,” explains Alexander Korsunsky. “Improving groundbreaking technology, such as wet cavitation peening, will allow the design of higher-performance, more reliable systems for power generation and propulsion.”

The contact established with the biopharmaceutical company Sosei Heptares in 2019 was concretized in a first collaboration that will likely yield experimental results in 2021. Sosei Heptares develops and produces G protein–coupled receptors (GPCRs) for structure-based drug design and targeted drug delivery. GPCRs are a large protein family of receptors and integral membrane proteins that activate cellular responses to external stimuli through numerous internal signal transduction pathways. Drugs developed for this human protein superfamily account for almost 40% of all prescription drugs on the market to date, yet structure-based drug design has never been deployed for this superfamily of receptors. During a workshop at European XFEL, the potential of X-ray FELs for GPCR research and development was discussed, and a basis of collaboration for the development of a suitable sample environment to collect data was established.

Regarding patents, ILO has informed the European XFEL staff scientists and engineers about intellectual property protection and subsequent exploitation. The first patent was filed and has received an evaluation, with a promising expectation of a grant. A further patent will be filed. Filing a patent involves additional work on top of the already demanding needs of fundamental scientific research, and therefore requires not only creativity and technical competence but also great dedication.

ILO helped to organize the Big Science Business Forum in Granada, Spain, which unfortunately had to be postponed until 2021. The event will bring together key suppliers and high-level representatives of various international science institutes, including European XFEL, to explore new possibilities for advancing the development of novel technologies. Moreover, a temporary innovation marketplace will be set up in order to foster technology transfer. Webinars were organized in 2020, while attendees waited for the in-person conference. In particular, a virtual event will take place in February 2021 to inform and promote the technology transfer track programme that will be held during the conference.

ILO was actively involved in various third-party–funded projects between industry and academia to exploit the potential synergy of these two worlds. ILO also participated in the monitoring of part of the 170 projects awarded in the framework of ATTRACT, a pioneering initiative bringing together European fundamental-research and industrial communities in order to lead to the next generation of detection and imaging technologies. Based on the ATTRACT results, ILO contributed to an in-depth study of the issues in the collaboration between industry and academia in order to improve it. Furthermore, ILO organized a workshop on the topic and collected input from different stakeholders in this environment.

A systematic process was started to evaluate the impact of European XFEL research and development activities on industry by combining data available from different groups, from scientific to administrative ones, for example Finance and Procurement. This monitoring will support the management in the decision-making in order to optimize the innovative impact of European XFEL basic research. Moreover, a template of a new ILO report has been drafted that makes it possible to access the highlights of cutting-edge components and technology, deliveredfrom the suppliers and industrial collaborations of European XFEL.

Figure 2: ZAL and Airbus representatives visited European XFEL and discussed laser peening as a possible application for characterization at the HED instrument. Picture taken in early 2020 before the lockdown.

Outreach

In 2020, European XFEL reached out to non-expert audiences predominantly via online activities. New digital resources were created and older ones updated. The virtual tour using 360° photographs was upgraded, implemented for reserved virtual visits, and made available online.

Communication support for scientific events included virtual tours of the facility as well as new videos featuring scientific group leaders. Two versions of these videos were produced: a longer one for expert audiences, with detailed explanations, and a shorter one, aimed at non-experts.

Outreach for schools continued with an online holiday event for Young Talents (YoTa) Hamburg and a virtual tour for the CERN programme “Beamline for Schools”. The YoTa event was live-streamed from the sample environment laboratories. Students got insights into both light and electron microscopy, with opportunities to ask questions and choose which samples to investigate in detail. The winning teams from “Beamline for Schools” participated in a hybrid beamtime at DESY, including a virtual tour of European XFEL. In January and February, around 400 individual visitors attended 13 guided tours of the facility. The visitors included university students, school classes, scientists, and local interest groups. As of March, all tours were moved online; however, many groups preferred to postpone their visit to a later date. Posters about European XFEL were displayed at the annual science festival “Highlights der Physik” in Würzburg and at a virtual event for postdocs returning to Germany. Other planned events were cancelled in response to the COVID-19 pandemic. Two online public lectures drew large audiences. The lecture on COVID-19 research, part of the DESY series “WissensWerte”, had about 200 viewers. A talk by Robert Feidenhans’l at the Chaos Computer Club’s annual conference drew roughly 800 people.

Images of arts projects that showcase the confluence of arts and science at European XFEL are now featured on dedicated webpages available to online visitors. Planning for the visitor and conference centre continued in 2020, with the architectural design of the building and detailed plans of the exhibition being developed. This new building will accommodate a greater number of visitors, including the general public, and allow high-school students to spend a full day at European XFEL and perform their own experiments. The visitor centre, which is scheduled to open its doors in 2023, will include seminar rooms, two school labs, and an exhibition area.

Figure 1:
In July 2020, the online event for Young Talents (YoTa) Hamburg was live-streamed from the sample environment laboratories.

Figure 2:
The art of science: A new webpage details European XFEL arts projects.

Figure 3: To mark the International Day for the Elimination of Violence against Women on 25 November 2020, the European XFEL main building and campus restaurant were illuminated in bright orange.

Director’s Outlook

The outlook for 2021 is still strongly affected by the pandemic situation. At the end of 2020, the COVID-19 pandemic grew again in strength and put large parts of Europe into lockdown. At the time of writing, lockdown measures in Germany and other parts of Europe are expected to be maintained until at least early summer 2021. As a result, the start of user experiments had to be postponed by up to two months.

In the spring of 2021, a number of COVID-19 related experiments are scheduled at the SPB/SFX instrument, followed by the start of user experiments at the other instruments. User experiments will resume in August after the summer shutdown, which will, as usual, be used for repairs and installing new instrumentation. We are optimistic that more users can be invited for the experiments scheduled in the fall than in the spring, but we still have to consider how situation due to the pandemic changes. It is essential to have good communication with the users, and having on-site presence is preferable. We hope that we can further increase scientific output by the end of the year. For 2022 we plan a significant increase in beamtime and user experiments as compared to the pre-crisis level in 2019.

We have used the period without user experiments to introduce two novelties: First, the experiments at the instruments will, in a test phase, be done in a mode of operation where beamtime to an instrument is dedicated on a weekly basis and not, as previously, on a 12-hour basis. Furthermore, in this phase, there is no support at night. Not having users on site puts a heavy extra burden on the instrument staff, and daytime-only support gives more robustness to the operation. In addition, it significantly reduces the time needed to switch the X-ray beam from one instrument to another and provides a much better flow to the experiments. Second, we introduced a Data Operation Centre (DOC) and a Data Run Coordinator. The DOC is the hotspot for all issues concerning data, controls, and detectors in order to secure optimum and fast support for the instruments. I look forward to learning what efficiencies these two new elements of operation will give the facility and the users. A first assessment will be done by the summer.

In the fall of 2020, a strategy process started in which the mission and vision statement of the facility was defined. During 2021, a detailed overall strategy on how to realize the vision will be put in place, expressing the ambitions for the facility, the experiment programme, and the user community. This is going to be an exciting process that will lay the foundation for the future of the facility.

An additional positive development during the pandemic: Our Science Seminar programme has really blossomed. Since speakers no longer have to travel, we have been able to line up a string of high-level speakers for the seminars. Likewise, we have attracted audiences from around the world. For some of the seminars, we have had more than 300 participants.

All in all, we miss personal contacts and unplanned discussions. I hope, in the second half of 2021, to see more users, our Council, and all of our committee members back on site.

FACTS AND FIGURES

Discussing facts and figures from 2020

At a Glance

The European XFEL is a research facility that opens up new research opportunities for science and industry. The 3.4 km long X-ray FEL generates ultrashort X-ray flashes for photon science experiments with a peak brilliance that is a billion times higher than that of the best synchrotron X-ray radiation sources.

Brilliant X-ray flashes for new research opportunities

With a repetition rate of up to 27 000 pulses per second and an outstanding peak brilliance, the world's largest X-ray laser produces ultrashort X-ray flashes that allow researchers to map the atomic details of viruses, decipher the molecular composition of cells, take three-dimensional images of the nanoworld, film chemical reactions, and study processes like those occurring deep inside planets.

The European XFEL is located mainly in tunnels 6 to 38 m underground. The 3.4 km long facility runs from the DESY research centre in Hamburg to the town of Schenefeld in the German federal state of Schleswig-Holstein (Figure 1).

The facility comprises three sites: the DESY-Bahrenfeld site with the injector complex, the Osdorfer Born site with one distribution shaft, and the Schenefeld campus site, which hosts the underground experiment hall with a large laboratory and office building on top. The latter serves as the company headquarters.

As of December 2020, 12 partner countries are member states of European XFEL: Denmark, France, Germany, Hungary, Italy, Poland, Russia, Slovakia, Spain, Sweden, Switzerland, and the United Kingdom. The international partners have entrusted the construction and operation of the facility to the non-profit European X-Ray Free-Electron Laser Facility GmbH, a limited liability company under German law. The company cooperates closely with its largest shareholder, DESY, a research centre of the Helmholtz Association, and with other organizations worldwide. The annual budget for the facility is approximately 132 million euro. The construction costs, including commissioning, amounted to 1.25 billion euro (at 2005 price levels). Currently, the host country, Germany (federal government, city–state of Hamburg, and state of Schleswig-Holstein) covers 58% of the costs. Russia contributes 27%, and each of the other international shareholders between 1% and 3%. To a great extent, the European XFEL facility was realized by means of in-kind contributions by shareholders and partners.

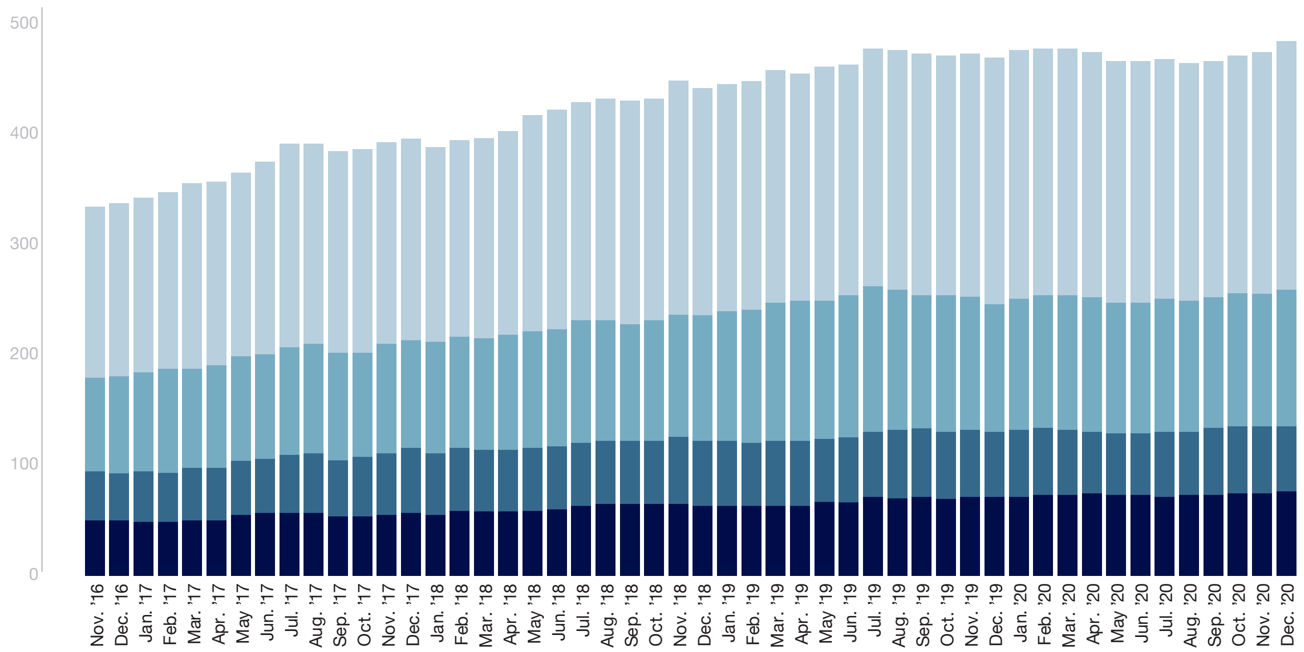
Aerial view of the European XFEL facility. Left to right: Schenefeld, Osdorfer Born, and DESY-Bahrenfeld sites.

Staff

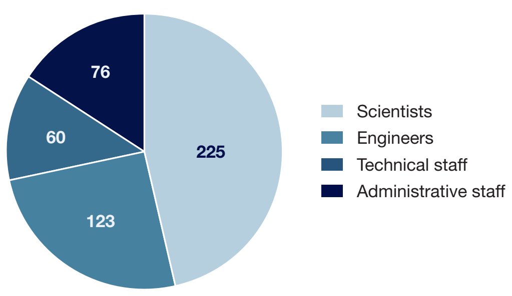
European XFEL employs staff members from 50 countries, bringing together various kinds of expertise to enable and support excellent and unique scientific research opportunities.

Staff development

Total headcount including guests and completed contracts: 484

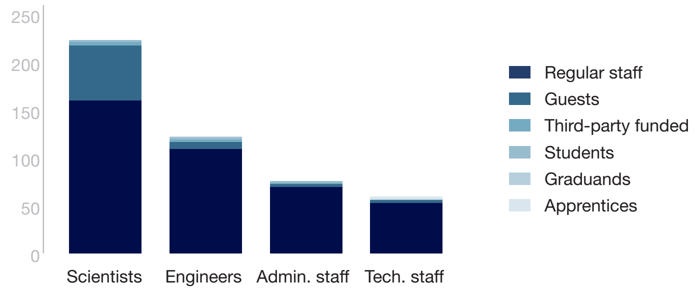


Functions

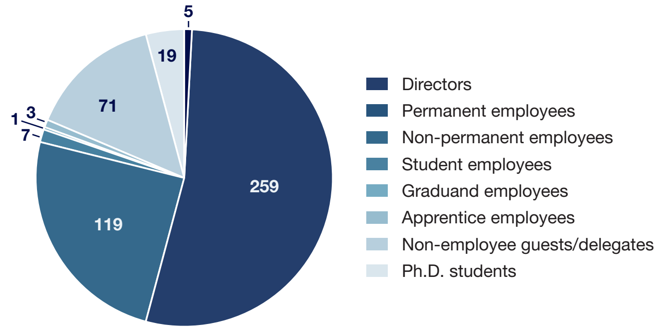


Contracts

Total staff, headcount

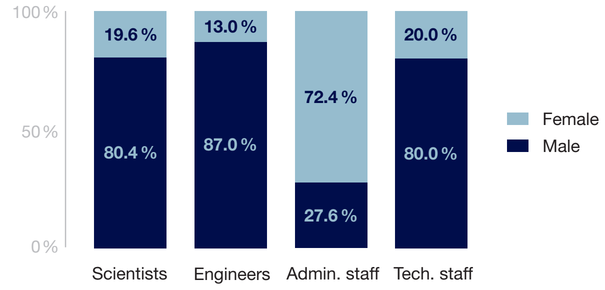


Contractual status



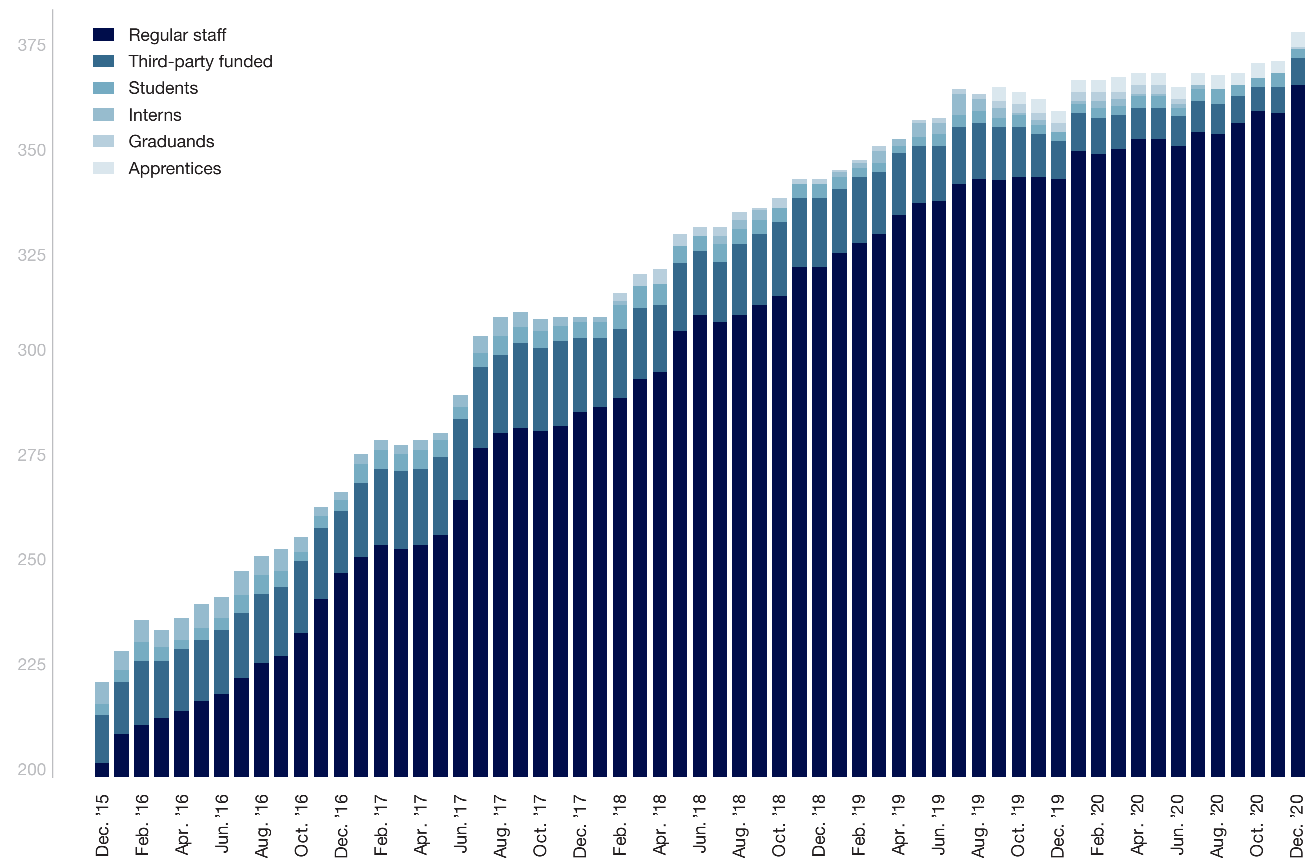
Gender ratio

Total share of women: 26.24%



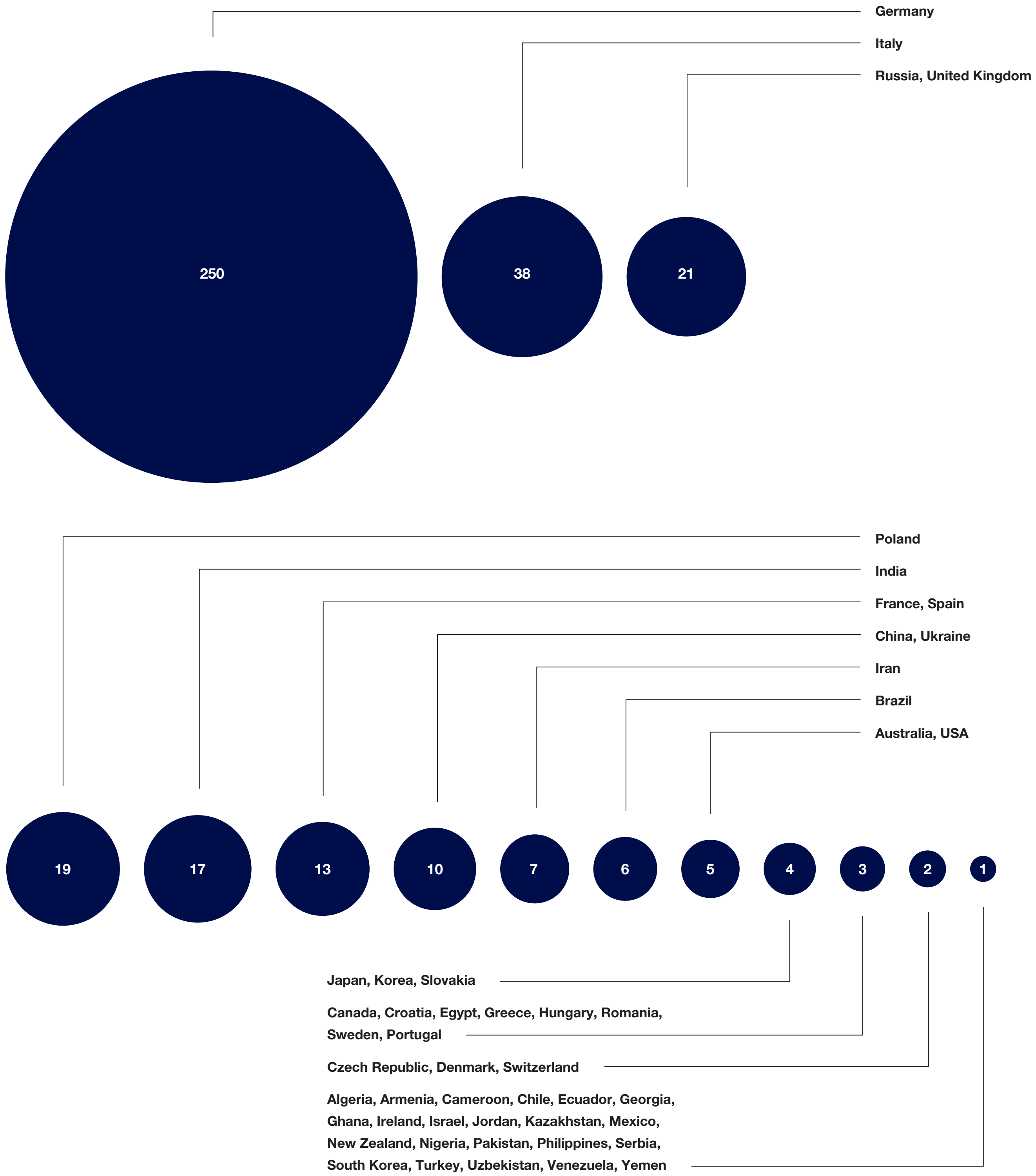
Full-time equivalents

Only actual European XFEL contracts: 387.32



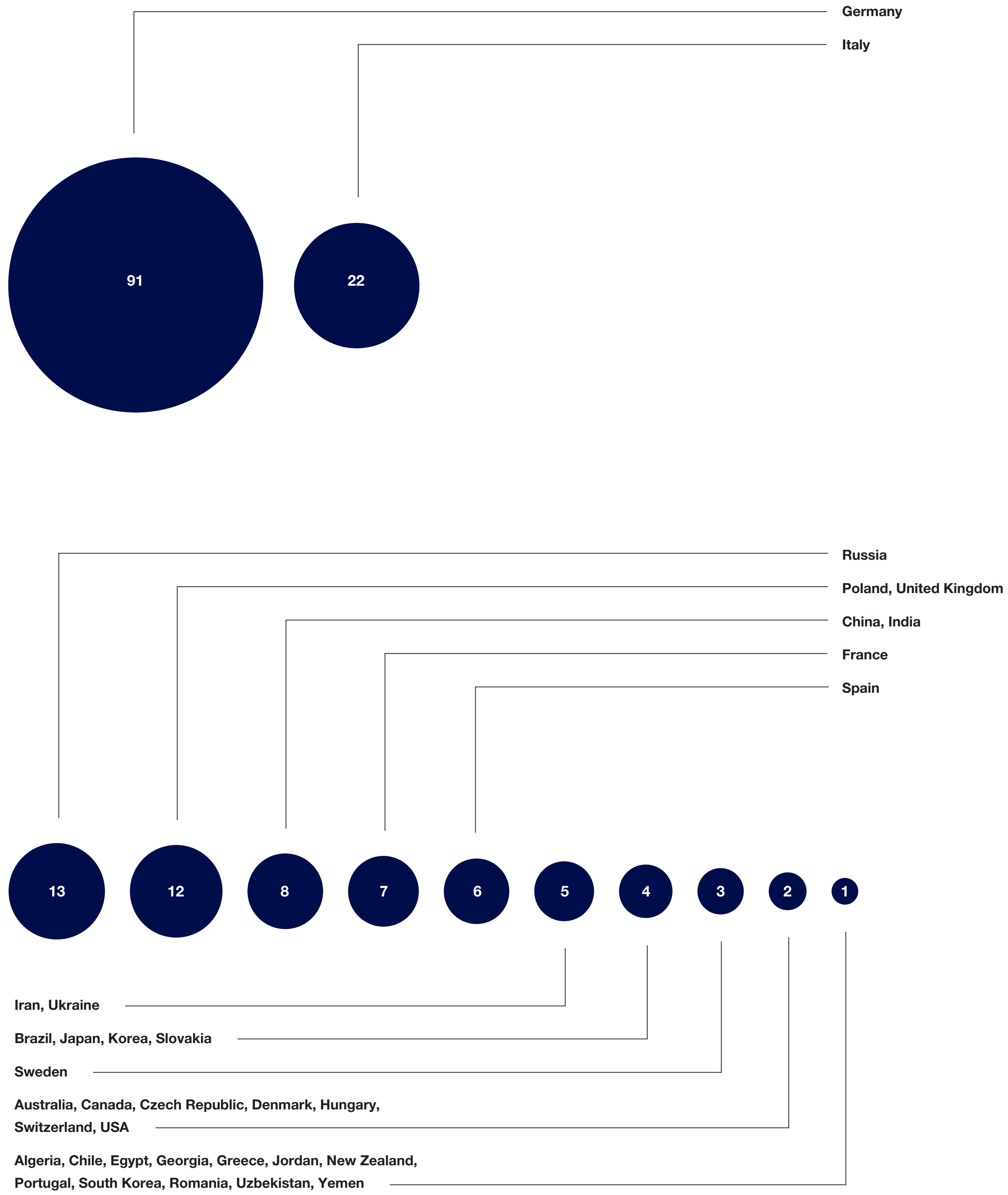
Total staff

50 citizenships in total, including 15 double citizenships



Scientific staff

34 citizenships in total, including 9 double citizenships



Shareholders

The European XFEL is organized as a non-profit company with limited liability under German private law (GmbH) that has international shareholders.

Member states	Present and likely (*) shareholders of the European XFEL GmbH
Denmark	**DAFHES** (Danish Agency for Higher Education and Science)
France	**CEA** (Commissariat à l'énergie atomique et aux énergies alternatives) **CNRS** (Centre national de la recherche scientifique)
Germany	**DESY** (Deutsches Elektronen-Synchrotron)
Hungary	**NRDI Office** (National Research, Development and Innovation Office)
Italy	**INFN** (Istituto Nazionale di Fisica Nucleare) **CNR** (Consiglio Nazionale delle Ricerche)
Poland	**NCBJ** (National Centre for Nuclear Research)
Russia	**NRC KI** (National Research Centre "Kurchatov Institute")
Slovakia	**Slovak Republic**
Spain*	Kingdom of Spain
Sweden	**VR** (Swedish Research Council)
Switzerland	**Swiss Confederation**
United Kingdom	**UKRI** (UK Research and Innovation)

The shareholders are designated by the governments of the member states, who commit themselves in an intergovernmental Convention to support the construction and operation of the European XFEL. In 2018, the Convention, which was originally signed in 2009, came into full effect.

Management, Council, and Committees

European XFEL Council

The European XFEL Council is the supreme organ of the company in which up to two delegates represent the shareholders of each member state. It meets at least twice a year. The Council functions as the shareholder assembly and decides on important issues of company policy.

Chairperson: **Maria Faury** (CEA, Paris)

Vice Chairperson: **Martin Meedom Nielsen** (DTU, Kongens Lyngby)

Delegates

Delegates	**Denmark**	**Morten Scharff** (DAFHES, Copenhagen)
	France	**Emmanuelle Lacaze** (CNRS, Paris) **Pascal Debu** (CEA, Paris)
	Germany	**Volkmar Dietz** (BMBF, Bonn) **Helmut Dosch** (DESY, Hamburg)
	Hungary	**Györgyi Juhász** (National Research, Development and Innovation Office, Budapest) **György Vankó** (Wigner Research Centre for Physics, Budapest)
	Italy	**Carlo Pagani** (INFN, Milan) **Corrado Spinella** (CNR, Rome)
	Poland	**Mateusz Gaczyński** (Ministry of Education and Science, Warsaw) **Ryszard Sobierajski** (Institute of Physics PAS, Warsaw)
	Russia	**Andrey Anikeev** until 31 August 2020 (Ministry of Science and Higher Education, Moscow) **Mikhail Kovalchuk** (NRC KI, Moscow)
	Slovakia	**Karel Saksl** (Institute of Materials Research, SAS, Košice) **Pavol Sovák** (P.J. Šafárik University, Košice)
	Sweden	**Lars Börjesson** (Chalmers University of Technology, Gothenburg) **Johan Holmberg** (VR, Stockholm)
	Switzerland	**Gabriel Aeppli** (PSI, Villigen) **Laurent Salzarulo** (SERI, Bern)
	United Kingdom	**Helen Beadman** (UKRI, Swindon) **James Naismith** (Rosalind Franklin Insitute, Didcot)
Observers	**Spain**	**Guadalupe C. de Córdoba Lasunción** (Ministerio de Ciencia e Innovación, Madrid)

Secretary: **Malte Laub** (European XFEL, Schenefeld, Germany)

Vice Secretary: **Meike Flammer** (European XFEL, Schenefeld, Germany)

Advisers

Germany	**Christian Harringa / Wim Leemans** (DESY, Hamburg)
	Sabine Carl (BMBF, Bonn)
Italy	**Federico Boscherini** (University of Bologna)
	Daniele Sertore (INFN, Milan)
Poland	**Zbigniew Gołębiewski** (NCBJ, Otwock-Świerk)
	Tomasz Leżański (NCBJ, Otwock-Świerk)
Slovakia	**Róbert Szabó** (Ministry of Education, Science, Research and Sport, Bratislava)
Switzerland	**Doris Wohlfender-Bühler** (SERI, Bern)
United Kingdom	**Amber Vater** (UKRI, Swindon)

Management Board

The European XFEL Management Board is composed of its chairperson and the administrative director, both acting as Managing Directors, and three scientific directors, acting also as proxy holders.

Chairperson and Managing Director — **Robert Feidenhans'l**

Managing and Administrative Director — **Nicole Elleuche**

Scientific Directors and Proxy Holders — **Serguei Molodtsov**, **Sakura Pascarelli**, **Thomas Tschentscher**

Administrative and Finance Committee

The Administrative and Finance Committee (AFC) is a committee of the European XFEL Council. It is charged with advising the Council on all matters of administrative issues and of financial management. The shareholders of each contracting party have a maximum of two representatives to the AFC. The chairperson and the vice chairperson of the AFC are appointed by the Council for a fixed period of two years.

Chairperson — **Xavier Reymond** (SERI, Bern, Switzerland)

Vice Chairperson — **Michał Wójtowicz** (NCBJ, Otwock-Świerk, Poland)

Delegates

Denmark	**Morten Scharff** (DAFHES, Copenhagen)
Germany	**Christian Harringa** (DESY, Hamburg)
	Sabine Carl since 20 February 2020 (BMBF, Bonn)
France	**Philippe Sassier** (CEA,Paris) and **Stéphanie Dupuis-Lê Vàn** (DSFIM, Paris)
Hungary	**Györgyi Kolossváryné Juhász** (NKFIH, Budapest)
Italy	**Veronica Buccheri** (INFN, Rome)
	Antonella Tajani (CNR, Rome)
Poland	**Michał Rybiński** (Ministry of Science and Higher Education, Warsaw)
Russia	**Valeriy Nosik** (NRC KI, Moscow)
Slovakia	**Pavol Sovák** (P.J. Šafárik University, Košice) and **Martin Šponiar** since 27 February 2020 (Ministry of Education, Science, Research and Sport, Bratislava)
Sweden	**Johan Holmberg** (VR, Stockholm)
	Hanifeh Khayyeri (VR, Stockholm)
Switzerland	**Peter Allenspach** (PSI, Villigen) and
	Doris Wohlfender-Bühler (SERI, Bern)
United Kingdom	**Rachel Reynolds** (STFC, Swindon)
	Amber Vater (UKRI, Swindon)

Secretary — **Uta Sprenger** (European XFEL, Schenefeld, Germany)

Vice Secretary — **Deike Pahl** (European XFEL, Schenefeld, Germany)

Machine Advisory Committee

The Machine Advisory Committee (MAC) advises the European XFEL Council and the Management Board in matters of fundamental importance regarding the accelerator complex.

Chairperson

Andrzej Wolski (University of Liverpool, UK)

Members

Camille Ginsburg (Jefferson Lab, Newport News, Virginia, USA)
Angeles Faus-Golfe (LAL, Orsay, France)
Evgeny Levichev (BINP, Novosibirsk, Russia)
Heung-Sik Kang (PAL, Pohang, South Korea)
Franz-Josef Decker (SLAC, Menlo Park, California, USA)
Luca Giannessi (Elettra Sincrotrone Trieste, Italy)
Peter Michel (HZDR, Dresden, Germany)
Thomas Schilcher (PSI, Villigen, Switzerland)
Catherine Madec (CEA, Paris)

Scientific Advisory Committee

The Scientific Advisory Committee (SAC) advises the European XFEL Council and the Management Board in scientific matters of fundamental importance. The SAC provides recommendations on all scientific, technical and policy issues that bear on a successful build-up of the scientific capacity of the European XFEL facility, its full and effective utilization as well as on future developments required to maintain the scientific and technical productivity of the facility at the highest possible level.

Chairperson

Ian Robinson Chair (UCL, London, UK)

Members

Olga Alekseeva (IC RAS, Moscow, Russia)
Michael Dunne (LCLS, Menlo Park, California, USA)
Stefan Eisebitt (MBI, Berlin, Germany)
Guillaume Fiquet (IMPMC, Paris, France)
Elspeth Garman (University of Oxford, UK)
Gerhard Grübel (DESY, Hamburg, Germany)
Steve Johnson (ETH, Zürich, Switzerland)
Maya Kiskinova (Elettra Sincrotrone Trieste, Italy)
Inari Kursula (University of Bergen, Norway, and University of Oulu, Finland)
Henrik Lemke (PSI, Villigen, Switzerland)
Anne l'Huillier (Lund University, Sweden)
Claudio Maschiovecchio (Elettra Sincrotrone Trieste, Italy)
Anders Nilsson (Stockholm University, Sweden)
Keith Nugent (The Australian National University, Australia)
Arwen Pearson (Universität Hamburg, Germany)
Alexander Popov (ESRF, Grenoble, France)
Christoph Quitmann (RI Research Instruments GmbH, Bergisch Gladbach, Germany)
Ilme Schlichting (MPI for Medical Research, Heidelberg, Germany)
Philippe Wernet (Uppsala University, Sweden)

Secretary

Gianluca Geloni (European XFEL, Schenefeld, Germany)

Detector Advisory Committee

The Detector Advisory Committee (DAC) for the European XFEL advises the SAC and, by extension, the company in all matters regarding the development of detectors needed to exploit the unique science opportunities of the facility.

Chairperson

Gabriella Carini (BNL, Upton, New York, USA)

Members

Branden Allen (Harvard College Observatory, Cambridge, Massachusetts, USA)
Jörn Wilms (University of Erlangen, Germany)
Paula Collins (CERN, Meyrin, Switzerland)
Andy Götz (ESRF, Grenoble, France)
Rob Halsall (STFC, Swindon, UK)
Mark Heron (Diamond Light Source, Oxford, UK)
Roland Horisberger (PSI, Villigen, Switzerland)
Michael Krumrey (PTB, Berlin, Germany)
Kay Rehlich (DESY, Hamburg, Germany)
Mark W. Tate (Cornell University, Ithaca, New York, USA)
Matthew Wing (UCL, London, UK)

Laser Advisory Committee

The Laser Advisory Committee (LAC) advises the DESY management, the European XFEL Management Board, and their relevant science committees in matters of research, development, and construction of the high-repetition-rate burst-mode laser systems used at the FLASH and European XFEL facilities.

Since a common technology platform is envisioned for these laser systems, DESY and European XFEL have decided to collaborate closely in their laser research and development efforts and to establish a common laser platform to which both institutes contribute. The committee consists of scientists not involved in the development activities.

Chairperson

Jonathan Zuegel (University of Rochester, New York, USA)

Members

Miltcho Danailov (Elettra Sincrotrone Trieste, Italy)
Thomas Dekorsy (DLR, Stuttgart, Germany)
Alan Fry (SLAC, Menlo Park, California, USA)
Patrick Georges (LULI, Palaiseau, France)
Catherine Le Blanc (Laboratoire LULI, Ecole Polytechnique, France)
Emma Springate (STFC Rutherford Appleton Laboratory, Didcot, UK)
William E. White (SLAC, Menlo Park, California, USA)

Secretaries

Nele Müller (DESY, Hamburg, Germany)
Jörg Hallmann (European XFEL, Schenefeld, Germany)

Proposal Review Panels

Access to beamtime for non-proprietary research at European XFEL is granted on the basis of peer review of scientific proposals. The Proposal Review Panels (PRPs) are in charge of the evaluation of the scientific merit of these proposals.

FXE Proposal Review Panel

Chairperson
Villy Sundström (Lund University, Sweden)

Vice Chairperson
Michael Wulff (ESRF, Grenoble, France)

Members
Shin-ichi Adachi (KEK, Tsukuba, Japan)
Frank de Groot (Utrecht University, The Netherlands)
Thomas Elsässer (MBI, Berlin, Germany)
Jerome Hastings (SLAC, Menlo Park, California, USA)
Adela Muñoz Páez (University of Sevilla, Spain)
Sylvain Ravy (Laboratoire de Physique des Solides, Orsay, France)
Alexander Soldatov (Southern Federal University, Rostov-on-Don, Russia)

HED Proposal Review Panel

Chairperson
Ryszard Sobierajski (Polish Academy of Sciences, Warsaw, Poland)

Vice Chairperson
Klaus Sokolowski-Tinten (University Duisburg-Essen, Germany)

Members
Michael Armstrong (LLNL, Livermore, California, USA)
Alessandra Benuzzi (LULI, Palaiseau, France)
Guillaume Fiquet (IMPMC, Paris, France)
Zahirul Islam (ANL, Lemont, Illinois, USA)
Matthias Marklund (Chalmers University, Gothenburg, Sweden)
David Neely (CLF, Didcot, UK)
Paul Neumayer (GSI, Darmstadt, Germany)
Norimasa Ozaki (Osaka University, Japan)
Sergey Pikuz (Joint Institute for High Temperatures, Moscow, Russia)

MID Proposal Review Panel (*)

Chairperson
Giulio Monaco (University of Padova, Italy)

Vice Chairperson
David Le Bolloc'h (Laboratoire de Physique des Solides, Orsay, France)

Members
Paul Fuoss (LCLS, Menlo Park, California, USA)
Henrik Lemke (PSI, Villigen, Switzerland)
Bridget Murphy (Christian-Albrechts-University, Kiel, Germany)
Anton Plech (KIT, Karlsruhe, Germany)
Ian Robinson (UCL, London, UK)
Anatoly Snigirev (Immanuel Kant Baltic Federal University, Kaliningrad, Russia)
Michael Sprung (DESY, Hamburg, Germany)

(*) A subset of the PRP was involved in COVID-19 MID Rapid-Access Reviews (June–August 2020)

SCS Proposal Review Panel

Chairperson
Jan-Erik Rubensson (Uppsala University, Sweden)

Vice Chairperson
Claudio Masciovecchio (Elettra Sincrotrone Trieste, Italy)

Members
Nicholas Brookes (ESRF, Grenoble, France)
Manuel Guizar-Sicairos (PSI, Villigen, Switzerland)
Philip Hofmann (University of Aarhus, Denmark)
Simo J. Huotari (University of Helsinki, Finland)
Steven Johnson (ETH, Zürich, Switzerland)
Alexey Kimel (Radboud University Nijmegen, Netherlands)
Maya Kiskinova (Elettra Sincrotrone Trieste, Italy)
Jan Lüning (HZB, Berlin, Germany)
Marcin Sikora (AGH University of Science and Technology, Krakow, Poland)

SPB/SFX Proposal Review Panel (**)

Chairperson
Inari Kursula (University of Bergen, Norway, and University of Oulu, Finland)

Vice Chairperson
Gyula Faigel (Wigner Research Centre for Physics, Budapest, Hungary)

Members
Sébastien Boutet (LCLS, Menlo Park, California, USA)
Elspeth Garman (University of Oxford, UK)
Cameron Kewish (Australian Synchrotron, Clayton, Australia)
Victor Lamzin (EMBL, Hamburg, Germany)
Thomas Möller (Technical University Berlin, Germany)
Christian Riekel (ESRF, Grenoble, France)
Jozef Uličný (P.J. Šafárik University, Košice, Slovakia)
Manfred Weiss (HZB, Berlin, Germany)

SQS Proposal Review Panel

Chairperson
Eckhardt Rühl (Freie Universität Berlin, Germany)

Vice Chairperson
John Costello (Dublin City University, Ireland)

Members
John D. Bozek (Synchrotron SOLEIL, Gif-sur-Yvette, France)
Carlo Callegari (Elettra Sincrotrone Trieste, Italy)
Alexei Grum-Grzhimailo (Lomonosov Moscow State University, Russia)
Jon Marangos (Imperial College London, UK)
Thomas Pfeifer (MPI for Nuclear Physics, Heidelberg, Germany)
Stacey L. Sorensen (Lund University, Sweden)
Frank Stienkemeier (University of Freiburg, Germany)
Linda Young (ANL, Lemont, Illinois, USA)
Beata Ziaja-Motyka (CFEL, Hamburg, Germany)

(**) A subset of the PRP was involved in COVID-19 SPB/SFX Rapid-Access Reviews (June–August 2020)

SCIENTIFIC RECORD

Attendees at the European XFEL Users' Meeting held in January 2020

Publications

User publications

An approach for the measurement of the bulk temperature of single crystal diamond using an X-ray free electron laser
A. Descamps et al.: Sci Rep **10** (1), 14564 (2020)
doi:10.1038/s41598-020-71350-x

Double Core-Hole Generation in O2 Molecules Using an X-Ray Free-Electron Laser: Molecular-Frame Photoelectron Angular Distributions
G. Kastirke et al.: Phys. Rev. Lett. **125** (16), 163201 (2020)
doi:10.1103/PhysRevLett.125.163201

Emergence of anomalous dynamics in soft matter probed at the European XFEL
F. Lehmkühler et al.: PNAS **117** (39), 24110–24116 (2020)
doi:10.1073/pnas.2003337117

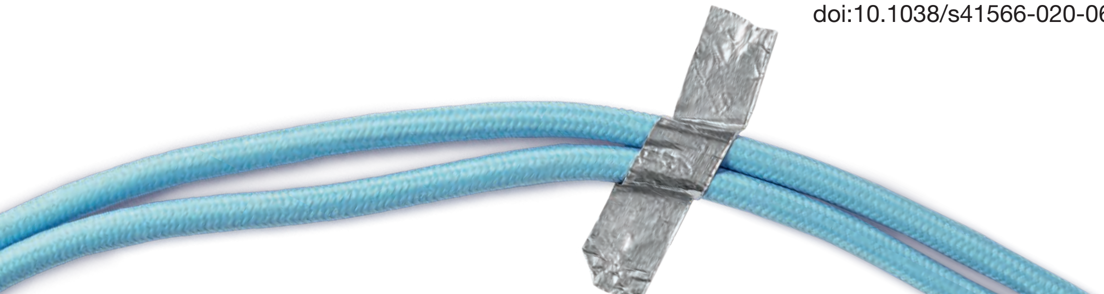
Exploring the light-induced dynamics in solvated metallogrid complexes with femtosecond pulses across the electromagnetic spectrum
M.A. Naumova et al.:
J. Chem. Phys. **152** (21), 214301 (2020)
doi:10.1063/1.5138641

Femtosecond X-ray emission study of the spin cross-over dynamics in haem proteins
D. Kinschel et al.: Nat. Commun. **11** (1), 4145 (2020)
doi:10.1038/s41467-020-17923-w

Mapping Resonance Structures in Transient Core-Ionized Atoms
T. Mazza et al.: Phys. Rev. X **10** (4), 041056 (2020)
doi:10.1103/PhysRevX.10.041056

Megahertz single-particle imaging at the European XFEL
E. Sobolev et al.: Commun. Phys. **3**, 97 (2020)
doi:10.1038/s42005-020-0362-y

Observation of fluctuation-mediated picosecond nucleation of a topological phase
F. Büttner et al.: Nat. Mater. **2020**, (2020)
doi:10.1038/s41563-020-00807-1



Photoelectron Diffraction Imaging of a Molecular Breakup Using an X-Ray Free-Electron Laser
G. Kastirke et al.: Phys. Rev. X **10** (2), 021052 (2020)
doi:10.1103/PhysRevX.10.021052

Photon-recoil imaging: Expanding the view of nonlinear x-ray physics
U. Eichmann et al.: Science **369** (6511), 1630–1633 (2020)
doi:10.1126/science.abc2622

Revealing Hot and Long-Lived Metastable Spin States in the Photoinduced Switching of Solvated Metallogrid Complexes with Femtosecond Optical and X-ray Spectroscopies
M.A. Naumova et al.:
J. Phys. Chem. Lett. **11** (11), 2133–2141 (2020)
doi:10.1021/acs.jpclett.9b03883

Segmented flow generator for serial crystallography at the European X-ray free electron laser
A. Echelmeier et al.: Nat Commun **11** (1), 4511 (2020)
doi:10.1038/s41467-020-18156-7

Shock Damage Analysis in Serial Femtosecond Crystallography Data Collected at MHz X-ray Free-Electron Lasers
A. Gorel et al.: Crystals **10** (12), 1145 (2020)

Spin cascade and doming in ferric hemes: Femtosecond X-ray absorption and X-ray emission studies
C. Bacellar et al.: PNAS **117** (36), 202009490 (2020)
doi:10.1073/pnas.2009490117

Time-resolved serial femtosecond crystallography at the European XFEL
S. Pandey et al.: Nat. Methods **17** (1), 73–78 (2020)
doi:10.1038/s41592-019-0628-z

Staff publications

A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator
W. Decking et al.: Nat. Photonics **391–397**, (2020)
doi:10.1038/s41566-020-0607-z

A portable on-axis laser-heating system for near-90° X-ray spectroscopy: application to ferropericlase and iron silicide
G. Spiekermann et al.:
J. Synchrotron Radiat. **27** (2), 414–424 (2020)
doi:10.1107/S1600577519017041

Acceleration of Crystallization Kinetics in Ge-Sb-Te-Based Phase-Change Materials by Substitution of Ge by Sn
P. Zalden et al.: Adv. Funct. Mater. **2020**, 2004803 (2020)
doi:10.1002/adfm.202004803

Amplified spontaneous emission in the extreme ultraviolet by expanding xenon clusters
A. Benediktovitch et al.:
Phys. Rev. A **101** (6), 063412 (2020)
doi:10.1103/PhysRevA.101.063412

An advanced workflow for single-particle imaging with the limited data at an X-ray free-electron laser
D. Assalauova et al.: IUCrJ **7** (6), 1102–1113 (2020)
doi:10.1107/S2052252520012798

An approach for the measurement of the bulk temperature of single crystal diamond using an X-ray free electron laser
A. Descamps et al.: Sci Rep **10** (1), 14564 (2020)
doi:10.1038/s41598-020-71350-x

Attosecond pulse shaping using a seeded free-electron laser
P.K. Maroju et al.: Nature **2020**, 1–6 (2020)
doi:10.1038/s41586-020-2005-6

Autoionization dynamics of helium nanodroplets resonantly excited by intense XUV laser pulses
Y. Ovcharenko et al.: New J. Phys. **22** (8), 083043 (2020)
doi:10.1088/1367-2630/ab9554

Breakdown of frustrated absorption in x-ray sequential multiphoton ionization
S.-K. Son et al.: Phys. Rev. Research **2** (2), 023053 (2020)
doi:10.1103/PhysRevResearch.2.023053

Charge disproportionation and nano phase separation in *RSrNiO4*
H. Guo et al.: Sci Rep **10** (1), 18012 (2020)
doi:10.1038/s41598-020-74884-2

Compact setup for spin-, time-, and angle-resolved photoemission spectroscopy
K. Bühlmann et al.:
Rev. Sci. Instrum. **91** (6), 063001 (2020)
doi:10.1063/5.0004861

Comparative Evaluation of Surface Quality, Tool Wear, and Specific Cutting Energy for Wiper and Conventional Carbide Inserts in Hard Turning of AISI 4340 Alloy Steel
A.T. Abbas et al.: Materials **13** (22), 5233 (2020)
doi:10.3390/ma13225233

Creating a diverse international user facility
S. Pascarelli et al.: Nat Rev Phys **2** (2), 337–339 (2020)
doi:10.1038/s42254-020-0201-9

Cryogenic Liquid Jets for High Repetition Rate Discovery Science
C.B. Curry et al.: J. Vis. Exp. **159** (159), e61130 (2020)
doi:10.3791/61130

Current status and future opportunities for serial crystallography at MAX IV Laboratory
A. Shilova et al.:
J. Synchrotron Radiat. **27** (5), 1095–1102 (2020)
doi:10.1107/S1600577520008735

Delay-detune scan for longitudinal electron beam characterization at free-electron lasers
S. Serkez et al.:
Phys. Rev. Accel. Beams **23** (12), 122801 (2020)
doi:10.1103/PhysRevAccelBeams.23.122801

Design and performance characterisation of the HAPG von Hámos Spectrometer at the High Energy Density Instrument of the European XFEL
T. Preston et al.: JINST **15** (11), P11033 (2020)
doi:10.1088/1748-0221/15/11/P11033

Diffraction data from aerosolized Coliphage PR772 virus particles imaged with the Linac Coherent Light Source
H. Li et al.: Scientific Data **7** (1), (2020)
doi:10.1038/s41597-020-00745-2

Direct observation of nuclear reorganization driven by ultrafast spin transitions
Y. Jiang et al.: Nat. Commun. **11** (1), 1530 (2020)
doi:10.1038/s41467-020-15187-y

Double Core-Hole Generation in *O2* Molecules Using an X-Ray Free-Electron Laser: Molecular-Frame Photoelectron Angular Distributions
G. Kastirke et al.: Phys. Rev. Lett. **125** (16), 163201 (2020)
doi:10.1103/PhysRevLett.125.163201

Double grating shearing interferometry for X-ray free-electron laser beams
M. Makita et al.: Optica **7** (5), 404–409 (2020)
doi:10.1364/OPTICA.390601

Double-pulse speckle contrast correlations with near Fourier transform limited free-electron laser light using hard X-ray split-and-delay
W. Roseker et al.: Sci. Rep. **10** (1), 5054 (2020)
doi:10.1038/s41598-020-61926-y

Dual boson diagrammatic Monte Carlo approach applied to the extended Hubbard model
M. Vandelli et al.: Phys. Rev. B **102** (19), 195109 (2020)
doi:10.1103/PhysRevB.102.195109

Dynamically pre-compressed hydrocarbons studied by self-impedance mismatch
N.J. Hartley et al.:
Matter Radiat. Extremes **5** (2), 028401 (2020)
doi:10.1063/1.5130726

Effects of orientation, lattice defects and temperature on plasticity and phase transition in ramp-compressed single crystal iron
N. Amadou et al.: Comput. Mater. Sci. **172**, 109318 (2020)
doi:10.1016/j.commatsci.2019.109318

Emergence of anomalous dynamics in soft matter probed at the European XFEL
F. Lehmkühler et al.: PNAS **117** (39), 24110–24116 (2020)
doi:10.1073/pnas.2003337117

Equation of state and high-pressure phase behaviour of *$SrCO_3$*
N. Biedermann et al.:
Eur. J. Mineral. **32** (6), 575–586 (2020)
doi:10.5194/ejm-32-575-2020

Evaluation of cobalt complexes with tripod ligands for zinc finger targeting
H.M. Aðalsteinsson et al.:
Dalton Trans. **49**, 16143-16153 (2020)
doi:10.1039/D0DT00067A

Evidence of shock-compressed stishovite above 300 GPa
M.O. Schoelmerich et al.: Sci. Rep. **10** (1), 10197 (2020)
doi:10.1038/s41598-020-66340-y

Exactly solvable model of strongly correlated *d*-wave superconductivity
M. Harland et al.: Phys. Rev. B **101** (4), 045119 (2020)
doi:10.1103/PhysRevB.101.045119

Exploring the light-induced dynamics in solvated metallogrid complexes with femtosecond pulses across the electromagnetic spectrum
M.A. Naumova et al.:
J. Chem. Phys. **152** (21), 214301 (2020)
doi:10.1063/1.5138641

Femtosecond electronic structure response to high intensity XFEL pulses probed by iron X-ray emission spectroscopy
R. Alonso-Mori et al.: Sci Rep **10** (1), 16837 (2020)
doi:10.1038/s41598-020-74003-1

Femtosecond laser produced periodic plasma in a colloidal crystal probed by XFEL radiation
N. Mukharamova et al.: Sci. Rep. **10** (1), 10780 (2020)
doi:10.1038/s41598-020-67214-z

Femtosecond timing synchronization at megahertz repetition rates for an x-ray free-electron laser
T. Sato et al.: Optica **7** (6), 716 (2020)
doi:10.1364/OPTICA.396728

Femtosecond X-ray emission study of the spin cross-over dynamics in haem proteins
D. Kinschel et al.: Nat. Commun. **11** (1), 4145 (2020)
doi:10.1038/s41467-020-17923-w

First Experiments in Structural Biology at the European X-ray Free-Electron Laser
G. Mills et al.: Appl. Sci. **10** (10), 3642 (2020)
doi:10.3390/app10103642

Full strain tensor measurements with X-ray diffraction and strain field mapping: a simulation study
M.X. Tang et al.:
J. Synchrotron Radiat. **27** (3), 646–652 (2020)
doi:10.1107/S1600577520003926

Gold Standard for macromolecular crystallography diffraction data
H.J. Bernstein et al.: IUCrJ **7** (5), (2020)
doi:10.1107/S2052252520008672

Growth of concomitant laser-driven collisionless and resistive electron filamentation instabilities over large spatiotemporal scales
C. Ruyer et al.: Nat. Phys. **16**, 983-988 (2020)
doi:10.1038/s41567-020-0913-x

Hard x-ray single-shot spectrometer at the European X-ray Free-Electron Laser
N. Kujala et al.: Rev. Sci. Instrum. **91** (10), 103101 (2020)
doi:10.1063/5.0019935

High-energy-resolution inelastic X-ray scattering spectrometer at beamline 30-ID of the Advanced Photon Source
A.H. Said et al.:
J. Synchrotron Radiat. **27** (3), 827–835 (2020)
doi:10.1107/S1600577520002854

High-pressure structural and electronic properties of *$CuMO_2$* (M=Cr, Mn) delafossite-type oxides
D. Levy et al.: Phys. Rev. B **101** (24), 245121 (2020)
doi:10.1103/PhysRevB.101.245121

Imaging plasma formation in isolated nanoparticles with ultrafast resonant scattering
D. Rupp et al.: Struct. Dyn. **7** (3), 034303 (2020)
doi:10.1063/4.0000006

Impact of real mirror profiles inside a split-and-delay unit on the spatial intensity profile in pump/probe experiments at the European XFEL
V. Kärcher et al.: J. Synchrotron Rad. **28** (1), online (2020)
doi:10.1107/S1600577520014563

***$K+$* vs. *$Na+$* Effects on the Self-Assembly of Guanosine 5´-Monophosphate: A Solution SAXS Structural Study**
E.J. Baldassarri et al.: Nanomaterials **10** (4), 629 (2020)
doi:10.3390/nano10040629

Laser-induced metastable mixed phase of AuNi nanoparticles: a coherent X-ray diffraction imaging study
Y. Kim et al.: J. Synchrotron Rad. **27** (3), 725–729 (2020)
doi:10.1107/S1600577520001617

Mapping Resonance Structures in Transient Core-Ionized Atoms
T. Mazza et al.: Phys. Rev. X **10** (4), 041056 (2020)
doi:10.1103/PhysRevX.10.041056

Mapping the emergence of molecular vibrations mediating bond formation
J.G. Kim et al.: Nature **582** (7813), 520–524 (2020)
doi:10.1038/s41586-020-2417-3

Megahertz single-particle imaging at the European XFEL
E. Sobolev et al.: Commun. Phys. **3**, 97 (2020)
doi:10.1038/s42005-020-0362-y

Microfluidic polyimide gas dynamic virtual nozzles for serial crystallography
M. Vakili et al.: Rev. Sci. Instrum. **91** (8), 085108 (2020)
doi:10.1063/5.0012806

Microfluidic synthesis of thermo-responsive block copolymer nano-objects via RAFT polymerization
T.E. Glier et al.: J Polym Res **27** (11), 333 (2020)
doi:10.1007/s10965-020-02290-3

Mirror to measure small angle x-ray scattering signal in high energy density experiments
M. Šmíd et al.: Rev. Sci. Instrum. **91** (12), 123501 (2020)
doi:10.1063/5.0021691

Monitoring laser-induced magnetization in FeRh by transient terahertz emission spectroscopy
N. Awari et al.: Appl. Phys. Lett. **117** (12), 122407 (2020)
doi:10.1063/5.0019663

New Method for Measuring Angle-Resolved Phases in Photoemission
D. You et al.: Phys. Rev. X **10** (3), 031070 (2020)
doi:10.1103/PhysRevX.10.031070

Noble metal nanoparticles in organic matrix
O. Molodtsova et al.: Appl. Surf. Sci. **506**, 144980 (2020)
doi:10.1016/j.apsusc.2019.144980

Novel method for the generation of stable radiation from free-electron lasers at high repetition rates
S. Ackermann et al.:
Phys. Rev. Accel. Beams **23** (7), (2020)
doi:10.1103/PhysRevAccelBeams.23.071302

Observation of fluctuation-mediated picosecond nucleation of a topological phase
F. Büttner et al.: Nat. Mater. **2020**, (2020)
doi:10.1038/s41563-020-00807-1

Opportunities for Two-Color Experiments in the Soft X-ray Regime at the European XFEL
S. Serkez et al.: Appl. Sci. **10** (8), 2728 (2020)
doi:10.3390/app10082728

Perspectives on single particle imaging with x-rays at the advent of high repetition rate x-ray free electron laser sources
J. Bielecki et al.: Struct. Dyn. **7** (4), 040901 (2020)
doi:10.1063/4.0000024

Phase separated bi-metallic PtNi nanoparticles formed by pulsed laser dewetting
K. Ahn et al.: Nanotechnology **32** (8), 085708 (2020)
doi:10.1088/1361-6528/abc9e9

Photoabsorption, photoionization, and Auger processes at the carbon edge in
R. Forbes et al.: Phys. Rev. A **101**, 023408 (2020)

Photoelectric effect with a twist
G. De Ninno et al.: Nat. Photonics **14** (9), 554–558 (2020)
doi:10.1038/s41566-020-0669-y

Photoelectron Diffraction Imaging of a Molecular Breakup Using an X-Ray Free-Electron Laser
G. Kastirke et al.: Phys. Rev. X **10** (2), 021052 (2020)
doi:10.1103/PhysRevX.10.021052

Photoelectron spectra and angular distribution in sequential two-photon double ionization in the region of autoionizing resonances of ArII and KrII
M.D. Kiselev et al.:
J. Phys. B: At. Mol. Opt. Phys. **53** (24), 244006 (2020)
doi:10.1088/1361-6455/abc2c5

Photoionization of the I 4d and valence orbitals of methyl iodide
R. Forbes et al.:
J. Phys. B: At. Mol. Opt. Phys. **53** (15), 155101 (2020)
doi:10.1088/1361-6455/ab8c5a

Photon-recoil imaging: Expanding the view of nonlinear x-ray physics
U. Eichmann et al.: Science **369** (6511), 1630–1633 (2020)
doi:10.1126/science.abc2622

Protein-crystal detection with a compact multimodal multiphoton microscope
Q.-d. Cheng et al.: Commun. Biol. **3** (1), 569 (2020)
doi:10.1038/s42003-020-01275-8

Pulsed electric fields induce modulation of protein liquid–liquid phase separation
M. Wang et al.: Soft Matter **16** (37), 8547–8553 (2020)
doi:10.1039/D0SM01478H

Real-space imaging of confined magnetic skyrmion tubes
M.T. Birch et al.: Nat. Commun. **11** (1), 1726 (2020)
doi:10.1038/s41467-020-15474-8

Resonant inelastic x-ray scattering on *CO2*: Parity conservation in inversion-symmetric polyatomics
J. Söderström et al.:
Phys. Rev. A **101** (6), 062501 (2020)
doi:10.1103/PhysRevA.101.062501

Revealing Hot and Long-Lived Metastable Spin States in the Photoinduced Switching of Solvated Metallogrid Complexes with Femtosecond Optical and X-ray Spectroscopies
M.A. Naumova et al.:
J. Phys. Chem. Lett. **11** (11), 2133–2141 (2020)
doi:10.1021/acs.jpclett.9b03883

Segmented flow generator for serial crystallography at the European X-ray free electron laser
A. Echelmeier et al.: Nat Commun **11** (1), 4511 (2020)
doi:10.1038/s41467-020-18156-7

Shock Damage Analysis in Serial Femtosecond Crystallography Data Collected at MHz X-ray Free-Electron Lasers
A. Gorel et al.: Crystals **10** (12), 1145 (2020)

Silver ion bioreduction in nanoparticles using Artemisia annua L. extract: characterization and application as antibacterial agents
A. Aghajanyan et al.: AMB Expr **10** (1), 66 (2020)
doi:10.1186/s13568-020-01002-w

Single-shot temporal characterization of XUV pulses with duration from ~10 fs to ~350 fs at FLASH
R. Ivanov et al.:
J. Phys. B: At. Mol. Opt. Phys **53** (18), 184004 (2020)
doi:10.1088/1361-6455/ab9c38

Spin cascade and doming in ferric hemes: Femtosecond X-ray absorption and X-ray emission studies
C. Bacellar et al.: PNAS **117** (36), 202009490 (2020)
doi:10.1073/pnas.2009490117

The role of transient resonances for ultra-fast imaging of single sucrose nanoclusters
P.J. Ho et al.: Nat. Commun. **11** (1), 1–9 (2020)
doi:10.1038/s41467-019-13905-9

The role of ultrafast magnon generation in the magnetization dynamics of rare-earth metals
B. Frietsch et al.: Sci. Adv. **6** (39), eabb1601 (2020)
doi:10.1126/sciadv.abb1601

The TRIXS end-station for femtosecond time-resolved resonant inelastic x-ray scattering experiments at the soft x-ray free-electron laser FLASH
S. Dziarzhytski et al.: Struct. Dyn. **7** (5), 054301 (2020)
doi:10.1063/4.0000029

Thermomechanical response of thickly tamped targets and diamond anvil cells under pulsed hard x-ray irradiation
J. Meza-Galvez et al.:
J. Appl. Phys. **127** (19), 195902 (2020)
doi:10.1063/1.5141360

Time-resolved serial femtosecond crystallography at the European XFEL
S. Pandey et al.: Nat. Methods **17** (1), 73–78 (2020)
doi:10.1038/s41592-019-0628-z

Time-resolved site-selective imaging of predissociation and charge transfer dynamics: the *CH3I* B-band
R. Forbes et al.:
J. Phys. B: At. Mol. Opt. Phys **53** (22), 224001 (2020)
doi:10.1088/1361-6455/abb1fd

Time-Resolved XUV Opacity Measurements of Warm Dense Aluminum
S. Vinko et al.: Phys. Rev. Lett. **124** (22), (2020)
doi:10.1103/PhysRevLett.124.225002

Tracking the ultraviolet-induced photochemistry of thiophenone during and after ultrafast ring opening
S. Pathak et al.: Nat. Chem. **12**, (2020)
doi:10.1038/s41557-020-0507-3

Transition regime in the ultrafast laser heating of solids
R. Shayduk et al.: J. Appl. Phys. **127** (7), 073101 (2020)
doi:10.1063/1.5143717

Ultracompact 3D microfluidics for time-resolved structural biology
J. Knoška et al.: Nat. Commun. **11** (1), 657 (2020)
doi:10.1038/s41467-020-14434-6

Ultrafast dynamics of 2-thiouracil investigated by time-resolved Auger spectroscopy
F. Lever et al.:
J. Phys. B: At. Mol. Opt. Phys. **54** (1), 014002 (2020)
doi:10.1088/1361-6455/abc9cb

Ultrafast magnetism: The magneto-optical Kerr effect and conduction electrons
R. Gort et al.: Appl. Phys. Lett. **116** (11), 112404 (2020)
doi:10.1063/1.5143115

Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst
M. Wagstaffe et al.:
ACS Catal. **10** (22), 13650–13658 (2020)
doi:10.1021/acscatal.0c04098

Ultrafast X-Ray Photochemistry at European XFEL: Capabilities of the Femtosecond X-Ray Experiments (FXE) Instrument
D. Khakhulin et al.: Appl. Sci. **10** (3), 995 (2020)
doi:10.3390/app10030995

Utilization of RADFET sensors for x-ray undulators: experiential considerations on magnetic field profile before commissioning
U. Englisch et al.:
Meas. Sci. Technol. **31** (11), 115902 (2020)
doi:10.1088/1361-6501/ab90bd

Visualizing Energy Transfer at Buried Interfaces in Layered Materials Using Picosecond X–Rays
C. Nyby et al.: Adv. Funct. Mater. **30** (34), 2002282 (2020)
doi:10.1002/adfm.202002282

Volt-per-Ångstrom terahertz fields from X-ray free-electron lasers
T. Tanikawa et al.:
J. Synchrotron Rad. **27** (3), 796–798 (2020)
doi:10.1107/S1600577520004245

X-ray detection of ultrashort spin current pulses in synthetic antiferromagnets
C. Stamm et al.: J. Appl. Phys. **127** (22), 223902 (2020)
doi:10.1063/5.0006095

X-ray diffraction from strongly bent crystals and spectroscopy of X-ray free-electron laser pulses
V.M. Kaganer et al.: Acta Cryst. A **76** (1), (2020)
doi:10.1107/S2053273319014347

X-ray diffractive imaging of controlled gas-phase molecules: Toward imaging of dynamics in the molecular frame
T. Kierspel et al.: J. Chem. Phys. **152** (8), 084307 (2020)
doi:10.1063/1.5133963

X-ray Spectroscopic Studies of a Solid-Density Germanium Plasma Created by a Free Electron Laser
G. Pérez-Callejo et al.: Appl. Sci. **10** (22), 8153 (2020)
doi:10.3390/app10228153

π -anisotropy: A nanocarbon route to hard magnetism
T. Moorsom et al.:
Phys. Rev. B: Condens. Matter **101** (6), 060408(R) (2020)
doi:10.1103/PhysRevB.101.060408

Workshops and Seminars

29–31 JANUARY 2020
European XFEL Users' Meeting
DESY, Hamburg, and European XFEL, Schenefeld, Germany

The European XFEL Users' Meeting is an annual opportunity to strengthen the interaction between European XFEL and the scientific user community. The 2020 meeting included plenary sessions of European XFEL and DESY Photon Science, as well as focused satellite meetings, workshops, and a poster session. The scope of this meeting included progress and current status of the European XFEL, scientific highlights from all six European XFEL instruments, instrument design developments and commissioning, and current developments in the field of X-ray FEL facilities.

Figure 2: Managing Director Robert Feidenhans'l welcomes the attendees of the European XFEL Users' Meeting

Figure 3: The poster session of the jointly organized Users' Meeting on 31 January 2020

Figure 1: Attendees of the MID Workshop "First year of operation and future developments" during the European XFEL Users' Meeting on 28 January 2020

Workshops

20–30 APRIL 2020
PaNOSC WP5 development sprint

This workshop included discussions about the ViNYL API development plan and collaborations with other PaNOSC work packages. Hands-on practice was also included. This project received funding from the European Union's Horizon 2020 research and innovation programme.

21–22 OCTOBER 2020
Toward liquid jet standardization at European XFEL

This workshop was aimed at international scientists as well as young scientists with an interest in liquid sample delivery systems at X-ray sources. The aim was to present the different injection devices available at the European XFEL and LCLS and to establish standards for the liquid jet environment.

11 NOVEMBER 2020
ATTRACT Task 3.3: Facilitate interaction with industrial partners

This workshop identified factors that have facilitated or impeded academy–industry interaction within the ATTRACT project. The goal was to elaborate a roadmap for possible improvements to the process for future open calls (outside of the scope of the current project).

10–11 DECEMBER 2020
Italy @ EuXFEL workshop

This workshop highlighted the scientific opportunities offered by the six instruments of the European XFEL, reviewed the interest of the Italian community in performing experiments at the European XFEL, and described practical steps to foster the links between European XFEL and the Italian user community. It was organized by the Italian Synchrotron Radiation Society (SILS) and European XFEL.

Seminars

Theory seminars

20 FEBRUARY
Modelling the evolution of X-ray-irradiated materials on femtosecond to nanosecond timescales
Vladimir Lipp, Center for Free-Electron Laser Science CFEL, DESY, Germany

12 MARCH
Infrared spectroscopy and dynamics of the Zundel and Eigencations by means of the multi-configurational time-dependent Hartree approach
Oriol Vendrell, Heidelberg University, Germany

15 APRIL
Clocking Auger electrons at XFELs
Nikolay M. Kabachnik, European XFEL, Germany, and Moscow State University, Russia

29 APRIL
Tracking the real-time changes of chemical bonds and electron dynamics
Antonio Picón, Autonomous University of Madrid, Spain

General seminars

6 MARCH
Interdisciplinary research beyond mainstream funding schemes: The Arab–German young academy of sciences and humanities
Jan Friesen, Department Catchment Hydrology, Helmholtz Centre for Environmental Research GmbH – UFZ, Germany

14 MAY
Informed Decision-making with new research opportunities for society
Paul Arthur Berkman, Director, Science Diplomacy Center, Fletcher School of Law and Diplomacy, Tufts University, Medford, Massachusetts, USA

9 JUNE
COVID-19 research opportunities and call for rapid access expressions of interest at European XFEL

COVID-19-related research opportunities at European XFEL and the open call for expressions of interest in rapid access were discussed during this online event hosted by the European XFEL User Organization Executive Committee (UOEC).

28 OCTOBER
hRIXS Virtual Town Hall Meeting
The current status of the hRIXS along with plans for commissioning and user operation were discussed at this virtual town hall meeting.

25 NOVEMBER
European XFEL Virtual User Information Meeting: 7th Call for Proposals
This meeting was hosted by the hosted by the European XFEL User Organization Executive Committee (UOEC).

Science seminars

7 JANUARY
Purifying electron spectra from noisy pulses with machine learning using synthetic Hamilton matrices
Jan-Michael Rost, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

21 JANUARY
Time-resolved diffraction experiments at X-ray free electron lasers reveal ultrafast structural changes in photosynthesis
Richard Neutze, Department of Chemistry and Molecular Biology, University of Gothenburg, Sweden

4 FEBRUARY
Ptychography - probing the limits of diversity
Pierre Thibault, Physics and Astronomy, University of Southampton, United Kingdom

20 FEBRUARY
Modelling the evolution of X-ray-irradiated materials on femtosecond to nanosecond timescales
Vladimir Lipp, Center for Free-Electron Laser Science (CFEL), DESY, Germany

3 MARCH
Laser ion acceleration using the Draco Petawatt facility at HZDR – plasma experiments and radiobiological application
Karl Zeil, Helmholtz-Zentrum Dresden-Rossendorf, Germany

12 MARCH
Infrared spectroscopy and dynamics of the Zundel and Eigencations by means of the multi-configurational time-dependent Hartree approach
Oriol Vendrell, Heidelberg University, Germany

31 MARCH
GSI and FAIR – Status and Prospects
Joerg Blaurock and Paolo Giubellino, GSI and FAIR, Darmstadt, Germany

14 APRIL
Spin cross-over dynamics and charge transfer in biology
Majed Chergui, LSU and LACUS, Lausanne, Switzerland

28 APRIL
Recent advances in light induced superconductivity
Andrea Cavalleri, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany, and Department of Physics, University of Oxford, United Kingdom

12 MAY
RIXS, phonons and charge density fluctuations
Giacomo Ghiringhelli, Dipartimento di Fisica, Politecnico di Milano, Italy

26 MAY
Advances in plasma accelerators and their future prospect
Wim Leemans, Accelerator Division, DESY, Germany

2 JUNE
Attosecond pulses by high-order harmonic generation in gases and attosecond spectroscopy
Anne L'Huillier, Atomic Physics, Lund University, Sweden

16 JUNE
FASTCORR – hopefully a strong partner to the research around XFEL in Hamburg
Olle Eriksson, Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

30 JUNE
Crystallography above 100 GPa: surprises and challenges
Leonid Dubrovinsky, BGI, University of Bayreuth, Germany

8 SEPTEMBER
Perspectives on single particle imaging at the LCLS
Andrew Lee Aquila, SLAC National Accelerator Laboratory, California, USA

22 SEPTEMBER
Mapping atomic motions with ultrabright electrons: fundamental space-time limits to imaging chemistry
R.J. Dwayne Miller, Departments of Chemistry and Physics, University of Toronto, Canada

6 OCTOBER
New research opportunities with FELs
Claudio Masciovecchio, Elettra Sincrotrone Trieste, Italy

27 OCTOBER
Attosecond science at the linac coherent light source
James P. Cryan, Stanford PULSE Institute, SLAC National Accelerator Laboratory, California, USA

17 NOVEMBER
Ultrafast modulation of order with coherent phonons: novel pathways to control of solids
Steven Johnson, Paul Scherrer Institute, Villigen, Switzerland

1 DECEMBER
Topological phase transitions and nonlinear interaction of X-rays with matter
Stefan Eisebitt, Max Born Institute, Berlin, Germany

Glossary

A

AGIPD
Adaptive Gain Integrating Pixel Detector
[European XFEL detector]

B

BMBF
Federal Ministry of Education and Research in Berlin, Germany

C

CCD
Charge-coupled device

CEA
Commissariat à l'énergie atomique et aux énergies alternatives in Saclay, France

CERN
European Council for Nuclear Research in Geneva, Switzerland

CFEL
Center for Free-Electron Laser Science in Hamburg, Germany

CNR
Consiglio Nazionale delle Ricerche in Rome, Italy

CNRS
Centre national de la recherche scientifique in Paris, France

D

DASTI
Agency for Science and Higher Education in Copenhagen, Denmark

DESY
Deutsches Elektronen-Synchrotron in Hamburg and Zeuthen, Germany

DSSC
Depleted P-Channel Field Effect Transistor Sensor with Signal Compression [European XFEL detector]

E

ESRF
European Synchrotron Radiation Facility in Grenoble, France

ETH Zürich
Eidgenössische Technische Hochschule in Zürich, Switzerland

F

FEL
Free-electron laser

FPH
FEL Physics Group

FXE
Femtosecond X-Ray Experiments
[European XFEL instrument]

H

HED
High Energy Density Science
[European XFEL instrument]

I

INFN
Istituto Nazionale di Fisica Nucleare in Rome, Italy

L

LCLS
Linac Coherent Light Source at SLAC in Menlo Park, California, USA

M

MEA
Maschinen- und Experimenteaufbau
[DESY group]

MID
Materials and Imaging Dynamics
[European XFEL instrument]

MKK
Maschine Kraft Kühlung Klima
[DESY group]

MVS
Maschinen Vakuum Systeme
[DESY group]

MXL
Group handling operation of the European XFEL facility and it's accelerator operated by DESY
[DESY group]

N

NCBJ
National Centre for Nuclear Research in Świerk, Poland

NKFIH/NRDI
National Research, Development and Innovation Office in Budapest, Hungary

P

PMO
Project management office

S

SASE
Self-amplified spontaneous emission

SCS
Spectroscopy and Coherent Scattering
[European XFEL instrument]

SLAC
SLAC National Accelerator Laboratory in Menlo Park, California, USA

SPB/SFX
Single Particles, Biomolecules, and Clusters and Serial Femtosecond Crystallography
[European XFEL instrument]

SQS
Small Quantum Systems
[European XFEL instrument]

T

TS
Technical Services

U

UKRI
UK Research and Innovation in Swindon, UK

UND
Undulator Systems

V

VR
Swedish Research Council in Stockholm, Sweden

X

XO
X-Ray Optics

XPD
X-Ray Photon Diagnostics

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Robert Feidenhans'l

Managing editor
Bernd Ebeling

Copy editors
Kurt Ament
Ilka Flegel, Textlabor, Kapellendorf
Misha Kidambi

Image editor
Frank Poppe

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Misha Kidambi

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European XFEL GmbH
Holzkoppel 4
22869 Schenefeld
Germany
+49 (0)40 8998-6006
contact@xfel.eu
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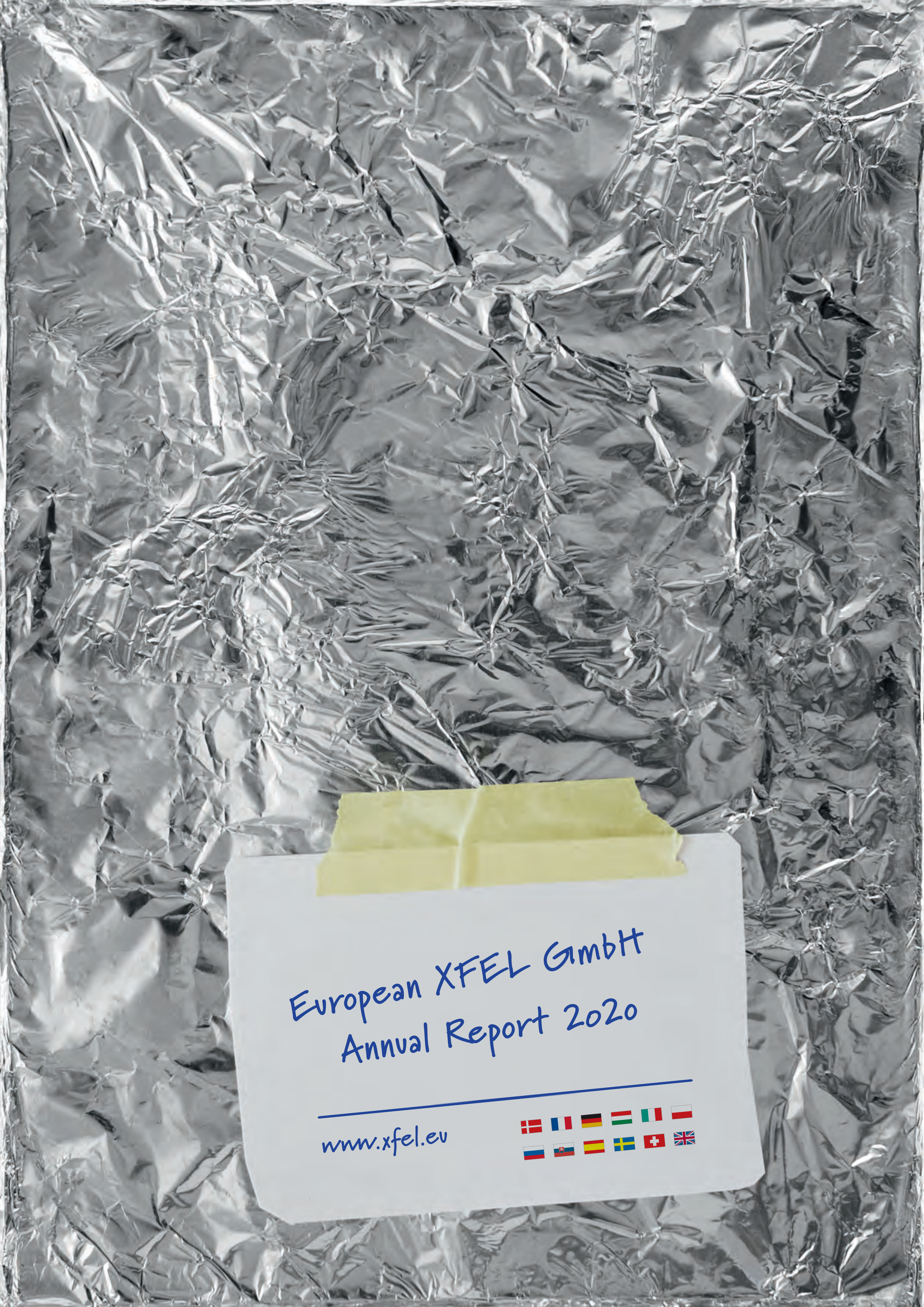
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