ANNUAL REPORT 2022

European XFEL

Developments, Results, Impressions

ANNUAL REPORT 2022

5 YEARS OF USER OPERATION

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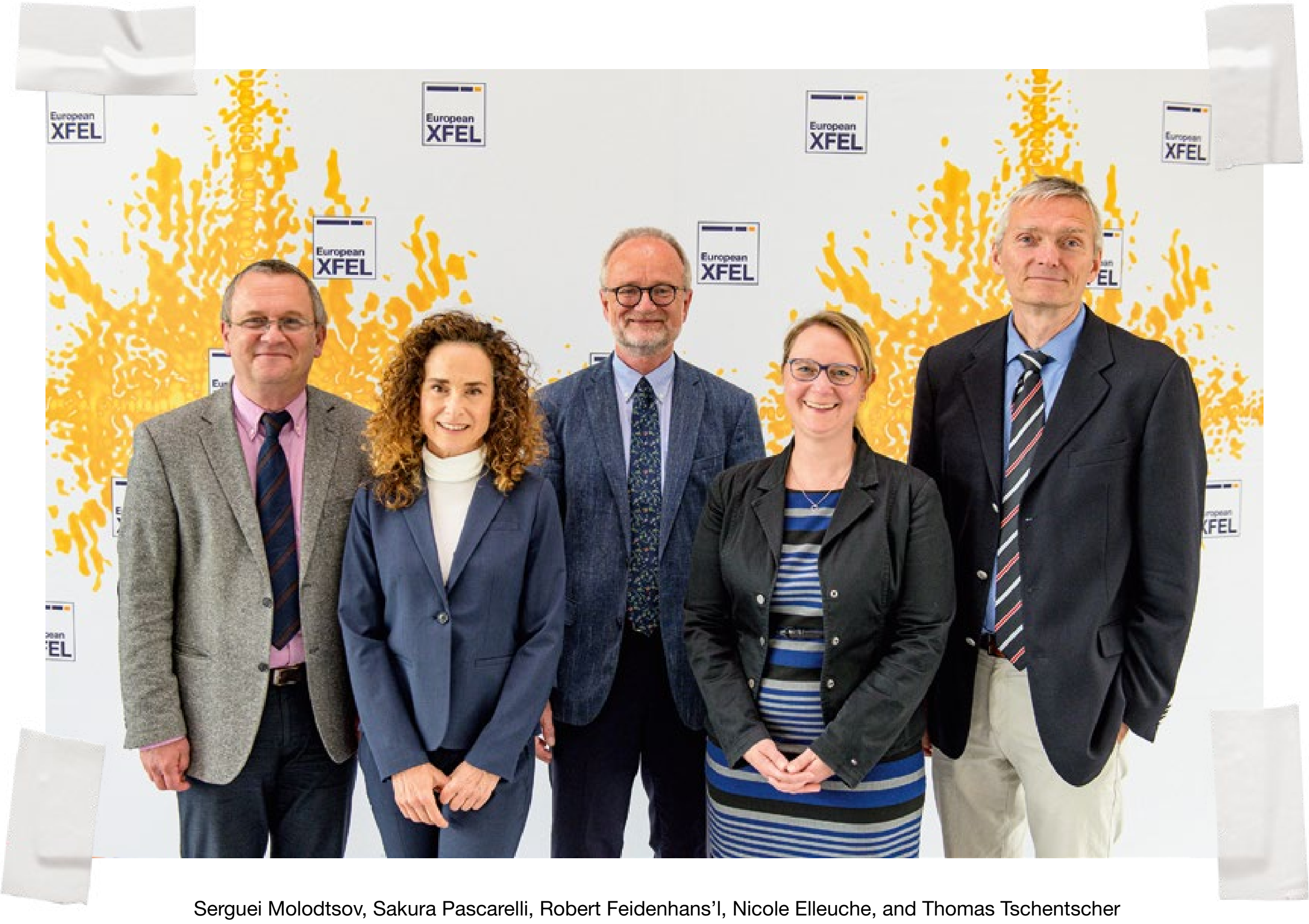
MANAGEMENT BOARD FOREWORD



Serguei Molodtsov, Sakura Pascarelli, Robert Feidenhans'l, Nicole Elleuche, and Thomas Tschentscher

The year 2022 was difficult for all of us, with the outbreak of war in Europe and the remnants of the COVID-19 pandemic posing challenges to the facility. However, we are pleased to report that we succeeded in overcoming and weathering many of the challenges the year brought with it.

Significant progress was made in the operation of the facility as well as in developing and enlarging the user programme. As a result of the joint efforts of our staff and the DESY accelerator team, the beamtime delivered to the user community nearly doubled, reaching more than 8100 hours in 2022. This was a massive step towards our goal of providing 10 500 hours per year by the second half of the decade. We also had 95 user experiments in 2022—close to double the number in 2021—and it was great to see many users come back on site with excellent and exciting research.

Other factors contributing to successful experiments were the control system, data analysis, and detectors, all of which further improved performance, as well as the Data Operation Centre, which once again showed its value.

In October, we celebrated the first five years of successful user operation, together with State Secretary Judith Pirscher from the German Federal Ministry of Education and Research and Deputy Mayor of Hamburg Katharina Fegebank. At the same time, we started the commissioning of our seventh scientific instrument, the Soft X-Ray Port (SXP). The new instrument will enable users to install and operate their own equipment, making way for new experimental opportunities.

Unfortunately, it is unlikely that 2022 will be remembered by our scientific community for these important milestones. Rather, it will be connected to the Russian invasion of Ukraine on 24 February. At European XFEL, all non-mandatory collaboration with Russia was halted, and researchers with Russian affiliations could no longer participate in experiments. Our guest house was opened to 30 refugees from Ukraine, and we were grateful to see the tremendous and overwhelming support for these refugees from our staff members with donations and personal assistance.

Finally, we would like to thank our Council and committees for their help and support, and welcome the new Council Chair, Federico Boscherini, whose expertise will be invaluable to the operation of the facility. We would also like to thank our fantastic users, who continue to do groundbreaking experiments at the European XFEL. In addition, we would like to express our gratitude to our colleagues at European XFEL and DESY for their commitment and enthusiasm, which have helped science and technology at our facility take another great step forward.

Robert Feidenhans'l **Nicole Elleuche**
Managing Directors

Serguei Molodtsov **Sakura Pascarelli** **Thomas Tschentscher**
Scientific Directors

COUNCIL CHAIR FOREWORD

I would like to start this short note by sharing with you that I feel truly honoured to serve as Council Chair of European XFEL, an outstanding and unique laboratory that is opening new areas of research in X-ray science and technology.

The year 2022, during which the fifth anniversary of successful user operation was celebrated, has brought considerable challenges to the company. The coronavirus pandemic has waxed and waned, a major geopolitical crisis with tragic consequences for innocent people erupted in Europe, and high inflation and soaring energy costs continue to challenge the financial landscape. However, I am sure that, with determination, caution, and collaboration among all stakeholders, we will weather the storm. The European XFEL community can count on my full commitment and the leadership that Council has entrusted in me.

Despite these difficulties, the user programme has proceeded in full swing with many users back on site. Exciting scientific results have been obtained, addressing four main societal challenges: Climate and Energy, Environment and Sustainability, Health, and Digitalization. New access modes have been implemented, with a very successful thematic call on water research. It is expected that other thematic calls will be opened in the future, while maintaining strong support for curiosity-driven research. Instrumental capabilities have also been expanded with first light achieved on the new Soft X-Ray Port (SXP) and the recent approval of the High-Energy X-Ray Scattering (HXS) instrument. The accelerator complex has performed very well, with new exciting developments relating to hard X-ray self-seeding, two-colour operation, and generation of sub-femtosecond pulses. The exploitation of the new capabilities and the science programme depend on the successful training of the next generation of scientists, supported by a strong Ph.D. programme—conducted in partnership with a number of European universities—which attracts a diverse student community.

The strategy process has been adjusted to the current times, and clear priorities have been identified that exploit the unique characteristics of the European XFEL facility: full development and use of self-seeding, the superconducting undulator radiation source, the HXS instrument, generation of sub-femtosecond pulses, a new generation of pixel detectors, and the preparation for the realization of the next two beamlines, SASE4 and SASE5. The European XFEL scientific community looks forward to the harvesting period in the next few years in which the great investment made will enable us to reap outstanding scientific results.

The financial outlook is causing great stress at many European large-scale facilities. We are therefore very happy that European XFEL has sufficient financial robustness to circumvent problems related to high energy costs without increased contributions from the shareholders in 2023. In fact, the 2023 budget was approved at the originally planned level.

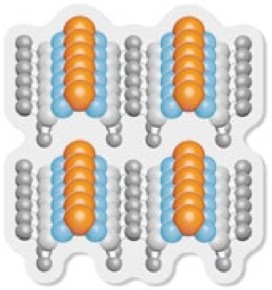
There are very positive developments concerning European XFEL governance. Nicole Elleuche's new contract as Administrative and Managing Director until March 2028 has been signed. The Chair of the Administrative and Finance Committee (AFC), Sabine Carl, has been re-appointed for her second term, and we are very grateful for the availability of Maja Hellsing as the new AFC Vice Chair starting in 2023.

During my first months of duty, it has been a pleasure to establish an excellent working relationship with the European XFEL Managing Directors, the Council Vice Chair, and the Council Secretariat. I would also like to thank our users and the European XFEL User Organization as well as the staff members of European XFEL and DESY for their excellent work and commitment. This is an excellent basis to face future challenges.

Federico Boscherini


HIGHLIGHTS
Light and X-rays interacting with a neon atom in a demonstration of record time resolution

SILVER SCREENING



New crystallography approach enables faster characterization of novel materials.

Technological innovation relies on novel materials. Industries require fast and effective characterization of such materials before integrating them into manufacturing processes. And yet, for many types of materials, this characterization can be slow and labour-intensive due to challenges in producing crystals for screening at X-ray sources. In a recent experiment at the FXE instrument, a group of scientists used a new crystallographic approach to study the structure of silver compounds from the material family known as "metal-organic chalcogenolates". The new approach opens the way to effective characterization of a wider range of materials.

New materials are the cornerstone of technological development. Innovation in a wide range of sectors—including renewable energy, transport, biotechnology, and information technology—is driven by new materials with improved characteristics. However, many such useful compounds are often found through fortuitous discovery rather than systematic design.

Understanding the fundamental structural and mechanical characteristics of compounds is key to developing new materials as part of a more conscious design process. Gaining such knowledge is often more difficult than it would appear. Crystallography techniques using X-rays are widely employed to study the 3D atomic arrangement of materials. However, crystallographic characterization remains a major bottleneck, as it can be difficult to grow crystals large enough to study with available light sources. In addition, there are few computational tools that can predict new, high-impact materials.

"With traditional characterization approaches, it can take years to screen and study new materials", says Christopher Milne, leading scientist at the FXE instrument of the European XFEL. "We need to find alternative ways of efficiently assessing potentially interesting materials and compounds. This is especially relevant in industries where we see rapid growth and innovation, such as in the development of quantum data technologies."

Compounds known as "metal-organic chalcogenolates" (MOChas) have recently attracted interest for their semiconducting properties and antimicrobial activity (Figure 1). These nanoconductors are of particular appeal for the field of quantum information science. However, because these materials produce nanocrystals or microcrystals, studying them with traditional X-ray crystallography techniques is extremely difficult, so there is a lack of knowledge about their atomic structure and understanding of how they function.

"In order to get enough detailed data from these tiny crystals using traditional X-ray light sources and crystallographic techniques, you need to illuminate them for such a significant length of time that you would destroy the crystal before you got your data", explains James Hohman from the University of Connecticut, USA, who led a recent experiment at FXE. "The extremely bright and precise X-rays generated by the European XFEL now give us the opportunity to develop new methods for characterization, ones that are not reliant on having large, stable crystals."

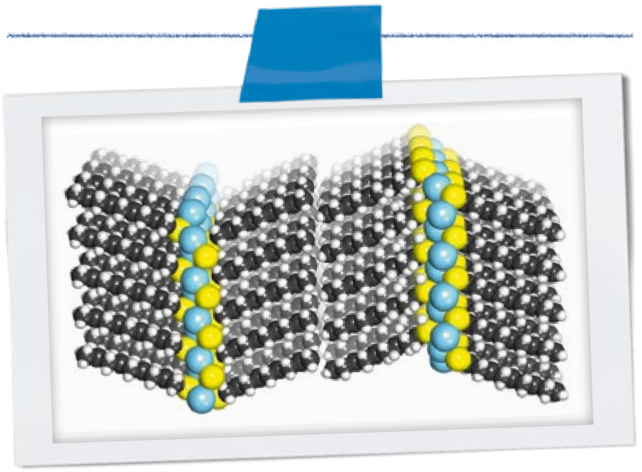


Figure 1: Space-filling perspective model depicting the general organization of silver (I) *n*-alkanethiolates, which are part of the MOChas family. The silver atoms are shown in blue and nominally arranged in a 2D layer, coordinated by sulphur atoms (yellow). The chains are packed end to end.

Taking an alternative approach to material characterization, Hohman, together with collaborators from across the globe, used a new technique, known as "small-molecule serial femtosecond X-ray crystallography" (smSFX), to study silver MOChas compounds. For their experiment, the scientists injected a liquid suspension of microcrystalline silver MOChas into the X-ray beam using a gas-dynamic virtual nozzle (GDVN). When an X-ray FEL pulse hits a crystal in the jet, an X-ray diffraction pattern is recorded, which allows a snapshot of the 3D arrangement of the atoms to be assembled after collecting many thousands of patterns (Figure 2). First results were extremely successful. The researchers solved the structures of three silver MOChas compounds at high resolution, revealing details of how the inorganic and organic components are layered.

While smSFX is very similar to its predecessor, serial femtosecond protein crystallography, two specific aspects of this technique are more demanding. "The ability of the FXE instrument to work at very short X-ray wavelengths of less than 1 Å and the possibility to position the LPD X-ray detector very close to the sample position were crucial for this technique to be successful", explains Milne. "This allowed us to collect diffraction peaks at very large scattering angles, which is necessary for the smSFX data analysis to be successful."

The experiment was a success. The uniquely high repetition rate of the X-ray pulses generated by the European XFEL resulted in extremely quick data collection. Around 6000 snapshots were captured in about two minutes, a feat that would take several hours at other X-ray FEL facilities. Furthermore, the very intense X-ray beam meant that the fine details of the compound structures could be observed, which is important for the identification of organic bonds in complex systems such as MOChas.

As the first experiment of its kind at the FXE instrument, the study was a large joint effort in terms of careful preparation and collaboration with many other groups for equipment integration, sample delivery, detector calibration, and implementation of the data analysis pipelines.

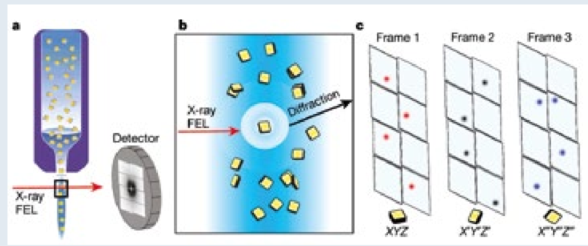


Figure 2: (a) Schematic of the smSFX experiment. (b) Randomly oriented microcrystals are delivered by GDVN into the interaction chamber and interact with the 30 fs X-ray pulses, producing diffraction images before being destroyed by the pulses. (c) Individual frames from randomly oriented crystals.

The scientists are now expanding the capabilities of this approach. As a next step, they plan to do time-resolved experiments, which are of significant interest for researchers studying light-sensitive chemicals used in materials such as photovoltaics.

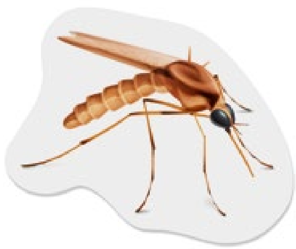
"Our breakthrough experiment demonstrated that smSFX can be applied as a general technique for structure determination of beam-sensitive nanocrystalline materials and, most importantly, of those with no reference structures available in structure databases", says Hohman. "Metal-organic chalcogenolates have been notoriously hard to study. Small-molecule femtosecond X-ray crystallography at the European XFEL has now opened the door to the investigation of this material family and others—an essential milestone for materials science."

Authors
M. Aleksich, D.W. Paley , E.A. Schriber, W. Linthicum, V. Oklejas, D.W. Mittan-Moreau, R.P. Kelly, P.A. Kotei, A. Ghodsi, R.G. Sierra, A. Aquilla, F. Poitevin, J.P. Blaschke, M. Vakili, C. Milne, F. Dall'Antonia, D. Khakhulin, F. Ardana-Lamas, F. Lima, J. Valerio, H. Han, T. Gallo, H. Yousef, O. Turkot, I.J. Bermudez Macias, T. Kluyver, P. Schmidt, L. Gelisio, A.R. Round, Y. Jiang, D. Vinci, Y. Uemura, M. Kloos, M. Hunter, A.P. Mancuso, B.D. Huey, L.R. Parent, N.K. Sauter, A.S. Brewster, J.N. Hohman

Reference
M. Aleksich et al.: submitted to J. Am. Chem. Soc. (2023)

The work on high-repetition SFX of crystalline hybrid solids was done as part of the user experiment #3073 (principal investigator J. Hohman). The experiment was carried out at the FXE instrument of the European XFEL.

STRUCTURAL INSIGHTS FOR IMPROVED CONTROL OF MOSQUITO-BORNE DISEASES



Two recent experiments reveal structural details of important bioinsecticides.

In tropical and subtropical regions, diseases transmitted by mosquitoes pose a significant burden to human health and social structures. Naturally crystalline mosquitocidal toxins isolated from soil bacteria are biodegradable and environmentally friendly and therefore have long been used as safe and effective tools for controlling mosquito populations. However, resistance against these natural toxins is emerging, raising concerns that they could become inefficient. A better understanding of the structure and function of these proteins is crucial for developing more effective bioinsecticides. Two recent experiments at the SPB/SFX instrument shed new light on the structure of toxins isolated from the bacteria *Bacillus thuringiensis* subsp. *israelensis* and *Lysinibacillus sphaericus*, providing clues about how to devise better treatments.

According to the World Health Organization (WHO), vector-borne diseases, including those transmitted by mosquitoes, account for around 17% of all infectious disease cases and more than 700 000 deaths every year worldwide [1].

Species from 3 of more than 50 known mosquito genera—*Anopheles*, *Aedes*, and *Culex*—are vectors for several life-threatening diseases. *Anopheles* mosquitoes transmit *Plasmodium* parasites that cause malaria, accounting for an estimated 247 million cases and over 600 000 deaths per year, mostly in children under five [2]. Dengue, a viral infection transmitted by *Aedes* mosquitoes, results in around 40 000 deaths each year. Other diseases include yellow fever, Zika, chikungunya (all three transmitted by *Aedes* mosquitoes), and West Nile fever (*Culex* mosquitoes).

Mosquito-borne diseases mostly occur in tropical and subtropical regions. However, a mix of environmental and demographic factors has been driving an expansion of the mosquitoes' range. Alongside medical treatment, vector control is a key element of strategies used by the WHO and local health authorities to reduce the burden of diseases transmitted by mosquitoes. Insecticides are sprayed and used to treat insect nets in areas where mosquitoes and associated diseases are prevalent. However, not only do chemical insecticides present a risk to human and ecosystem health, they also increase resistance in mosquitoes, meaning they are becoming less effective.

Naturally occurring nanocrystalline bioinsecticides offer a safer and more environmentally friendly option. Accordingly, mosquitocidal toxins isolated from the soil bacteria *Bacillus thuringiensis* subsp. *israelensis* and *Lysinibacillus sphaericus* have long been used as key components of bioinsecticides to control mosquito populations in plant crop protection. Combinations of proteins from these bacteria are used to increase the pathogenicity of such bioinsecticides. The proteins are toxic to only a small range of pests, including certain types of mosquito larvae, and are biologically degradable.

"Bioinsecticides are a key vector control measure in areas affected by diseases such as malaria", says European XFEL Scientific Director Sakura Pascarelli. "A better understanding of how proteins used in bioinsecticides actually affect mosquito larvae could help us determine how resistance occurs and enable the development of more effective and targeted products."

Figure 1: Two models showing possible structures of the Cry48Aa1–Tpp49Aa1 protein complex. Cry48Aa1 is represented in dark blue and Tpp49Aa1 in magenta. The region of Tpp49Aa1 that was experimentally shown to interact with Cry48Aa1 is indicated in green.

Although the toxicity and pesticidal qualities of these bioinsecticides have been appreciated and used for almost a century, little is known about their structure and exact function. "These proteins naturally form tiny crystals packed along with the bacterial spore, making them really difficult to study effectively with traditional crystallography methods", explains Colin Berry, Professor at Cardiff University in the UK, who led one of two recent experiments at the SPB/SFX instrument that studied the structure of such proteins. The crystals are so small that an extremely bright and tightly focused X-ray beam is needed to illuminate them enough so scientists can collect data of the quality required to resolve the atomic 3D structure of the proteins.

"The extremely bright and intense beam of the European XFEL gives us the unique opportunity to study these crystals *in situ*", explains Dominik Oberthür from the Center for Free-Electron Laser Science (CFEL), who, together with Berry and an international group of researchers, used serial femtosecond crystallography at SPB/SFX to study a protein known as Tpp49Aa1 that is found in the bacterium *Lysinibacillus sphaericus* [3]. "The beam could be focused to match the size of natural nanocrystals, and the beam intensity and the high repetition rate enabled us to collect a large set of high-quality data", adds first author Lainey Williamson, also from Cardiff University. The speed of the jet delivering the crystals was matched to the pulse rate of the intense X-ray beam so that tens of thousands of snapshots could be collected. The scientists then used these images to determine a 3D structural model of the protein.

The researchers not only determined the structure of the Tpp49Aa1 protein for the first time, they revealed significant details that enabled key insights into how the protein works. Using this data, the team went on to model the interaction of Tpp49Aa1 with another protein, Cry48Aa1, which interacts with it in bioinsecticides (Figure 1). The scientists also set up lab-based experiments to learn more about the pathogenicity of the protein pair.

The researchers are excited about the significance of the study. "We were able to show that this pair of proteins is actually toxic to more mosquito species than was previously realized", says Williamson.

In a second study [4], which also used serial femtosecond crystallography at the SPB/SFX instrument, scientists studied the two most potent mosquitocidal toxins produced by two subspecies of the soil bacterium *Bacillus thuringiensis (Bt):* Cry11Aa from *Bt* subsp. *israelensis* and Cry11Ba from *Bt* subsp. *jegathesan*. The two toxins differ in the spectrum of insects they affect and in the size of the crystals they form: Cry11Ba is more efficient against the *Aedes* mosquito and forms larger crystals than Cry11Aa. However, despite the importance and toxicity of these two proteins, little had been previously known regarding their structure. "The structures of these proteins had remained elusive because of their inability to recrystallize after extraction from the cells", explains Jacques-Philippe Colletier from the University of Grenoble Alpes in France, who led the study. "Furthermore, there was no known structural model of a related protein that could have been used as a reference in the structure building process."

In their experiment, Colletier and collaborators successfully solved the structure of these two proteins using a method known as "single-wavelength anomalous dispersion" (Figure 2). With this technique, a single dataset is collected to resolve a structural model without the use of reference models. "This is exciting because not only were the structures of these proteins completely unknown, they also have immediate relevance for mosquitocidal treatments", says Colletier. The data revealed the molecular basis for the unmatched toxicities of the two toxins, shedding light on how they could be further engineered to produce larger crystals or more potent toxins. Furthermore, the measurements, including those from three mutant toxin structures the scientists solved in addition to

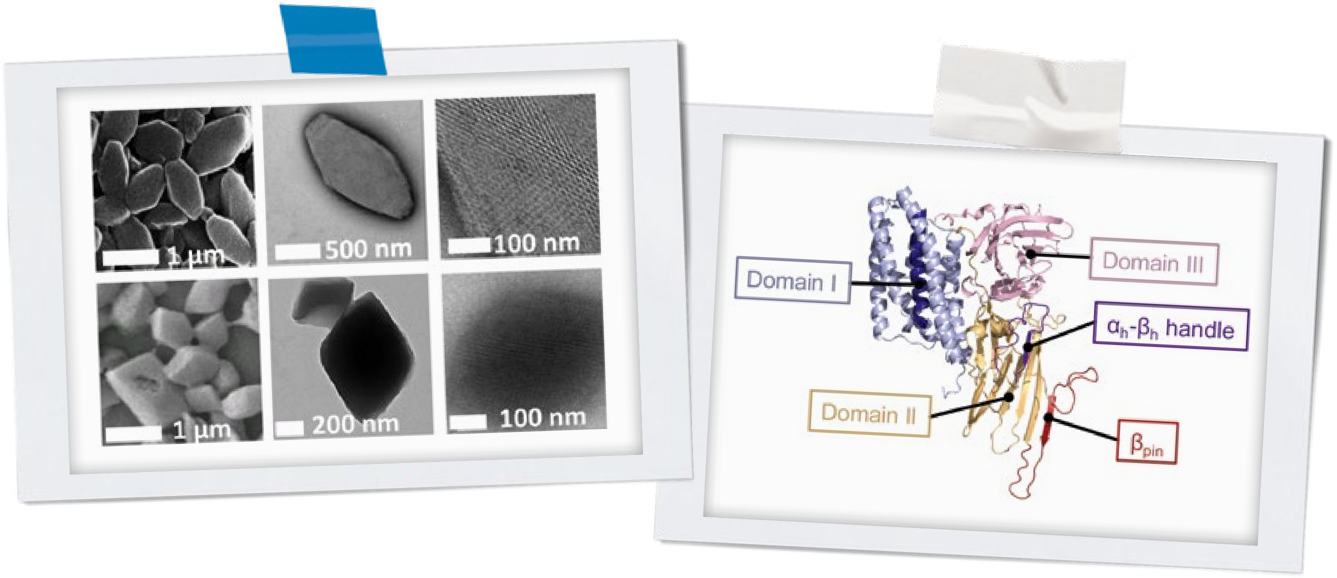


Figure 2:

Left: Crystals of the toxins Cry11Aa (top row) and Cry11Ba (bottom row). The panels show, from left to right, a scanning electron micrograph, a transmission electron micrograph, and a close-up view of the crystal surface.

Right: Determined structure of the Cry11Aa crystal. The different structural elements are indicated.

the two natural toxins, gave valuable insights into the crystallization process and how this might be controlled for effective toxin production. For example, by changing a single atom at a time in each of the two proteins—which are made up of around 7000 atoms each—it was possible to gain control of the shape, size, and dissolution properties of the nanocrystals, supporting the hypothesis that command can indeed be taken of the crystallization machinery of *Bacillus thuringiensis.*

“The ultimate goal of our research is to identify the structural determinants for the toxicity, spectrum, and *in vivo* crystallization of these naturally crystalline toxins”, explains Colletier. “We hope our research provides useful insights into how to produce new recombinant toxins that are endowed with improved toxicity and larger spectrum and that form bigger crystals. In this way, we may eventually reduce the costs associated with the production of bacterial mosquitocides and thus enable the use of *Bt*-derived mosquitocial products in developing countries.”

“These two projects have shown that, with the unique capabilities of its X-ray beam and instruments, the European XFEL can help to address some of the types of questions that have so far eluded structural biologists”, says Pascarelli. “The results will be extremely helpful in developing more effective vector control measures against some of the most devastating diseases across the world.”

Authors
First study:
L.J. Williamson, M. Galchenkova, H.L. Best, R.J. Bean, A. Munke, S. Awel, G. Pena, J. Knoska, R. Schubert, K. Dörner, E. Lloyd-Evans, M. Young, J. Valerio, M. Kloos, M. Sikorski, G. Mills, J. Bieleki, H. Kirkwood, C. Kim, R. de Wijn, K. Lorenzen, P.L. Xavier, A. Rahmani, L. Gelisio, O. Yefanov, A.P. Mancuso, H.N. Chapman, N. Crickmore, P.J. Rizkallah, C. Berry, D. Oberthür

Second study:
G. Tetreau, M.R. Sawaya, E. De Zitter, E.A. Andreeva, A.-S. Banneville, N.A. Schibrowsky, N. Coquelle, A.S. Brewster, M.L. Grünbein, G. Nass Kovacs, M.S. Hunter, M. Kloos, R.G. Sierra, G. Schiro, P. Qiao, M. Stricker, D. Bideshi, I.D. Young, N. Zala, S. Engilberge, A. Gorel, L. Signor, J.-M. Teulon, M. Hilpert, L. Foucar, J. Bielecki, R. Bean, R. de Wijn, T. Sato, H. Kirkwood, R. Letrun, A. Batyuk, I. Snigireva, D. Fenel, R. Schubert, E.J. Canfield, M.M. Alba, F. Laporte, L. Després, M. Bacia, A. Roux, C. Chapelle, F. Riobé, O. Maury, W. Li Ling, S. Boutet, A.P. Mancuso, I. Gutsche, E. Girard, T.R.M. Barends, J.-L. Pellequer, H.-W. Park, A.D. Laganowsky, J. Rodriguez, M. Burghammer, R.L. Shoeman, R.B. Doak, M. Weik, N.K. Sauter, B. Federici, D. Cascio, I. Schlichting, J.-P. Colletier

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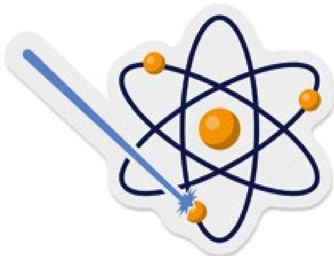
SETTING THE STAGE FOR ATTOSECOND SCIENCE AT THE EUROPEAN XFEL



First attosecond X-ray pulses at the European XFEL are measured directly in the time domain.

Attosecond X-ray science holds the key to studying electron dynamics from the vista of specific elements in matter. It thus promises to build the bridge between chemical and physical processes at the very onset of dynamics in matter after photoabsorption. And yet, even though facilities such as the European XFEL are on the verge of generating X-ray pulses that can be used to explore such processes in time-resolved experiments, actually measuring these attosecond pulses remains a cutting-edge challenge. In a recent experiment at the SQS instrument, scientists used a method known as “angular streaking” to non-destructively characterize all ultrashort X-ray pulses delivered to the instrument with attosecond resolution. This technique enabled them to pursue the first attosecond-resolved experiment at the European XFEL, targeting some of the fastest electron dynamics ever investigated with an X-ray laser.

The European XFEL can produce extremely short and intense X-ray pulses lasting only a few femtoseconds. These pulses are already being used to explore uncharted territory regarding fundamental physical phenomena, chemical reactions, and the atomic structures of biological molecules, such as proteins and viruses. While there is much more to discover in this femtosecond time range, the pulses’ stochastic substructure—which is due to the self-amplification of spontaneous emission in the SASE process—has remained unknown for the vast majority of experiments at X-ray FELs. This is one reason scientists are already looking to take the European XFEL one step further to reach an even briefer time scale—the attosecond time regime.

In a pioneering study at the SQS instrument, scientists from the SQS group, the FEL R&D group, and an international consortium around Wolfram Helml from TU Dortmund University and Markus Ilchen from DESY set out to characterize the ultrashort SASE pulses and use them to investigate some of the fastest electron dynamics ever targeted with X-rays. “A flurry of processes happens within a few femtoseconds, or even in a sub-femtosecond time window, after exposure to X-ray FEL photons, ultimately determining the response of matter to X-ray illumination”, explains Helml. “Without knowing the exact temporal structure of the X-ray pulses, one is practically blind to the important physical origins of the subsequently evolving dynamics.”

Attosecond X-ray science is expected to allow scientists to connect physical processes at the time scale of electronic movement with ultrafast chemical and molecular reactions. Just as the speed of a camera shutter needs to match the speed of the movement the photographer is trying to capture, so X-ray pulses that match the speed of these electronic, chemical, and structural processes on atomic scales enable scientists to study the details of these dynamics. However, while FEL technology can now provide attosecond X-ray pulses at the European XFEL, as demonstrated in this study, researchers can enter this new era of exploration only with detailed information from direct measurements of the exact time and energy structure of each X-ray pulse.

“The spikes of the SASE pulses in the X-ray regime have a duration typically on the order of a few hundreds of attoseconds, and the current generation of diagnostic methods struggles to routinely resolve these individual spikes", says Ilchen. "The temporal structure of the spikey X-ray FEL pulses determines the dynamical response of matter to the X-ray photons to a large extent in a broad variety of experiments, not only at SQS. The accurate characterization of each incoming pulse in real time is one of the most pressing technical challenges we face at FELs, particularly in opening up the field of attosecond X-ray science."

To characterize the SASE pulses, the scientists have developed a technique known as "angular streaking" [2]. For this method, X-ray pulses ionize a gas, in this case neon, which produces photoelectrons with well-defined characteristics. When the photoelectrons are generated in the presence of an external rotating optical laser field, they act as a clock. Their momenta are modified, leading to shifts in their kinetic energies and emission angles, which reveal the exact time the electrons are emitted and thus the spikey intensity structure of the X-ray FEL pulses. At SQS, the team used an advanced multi-spectrometer setup, consisting of 16 high-resolution time-of-flight electron spectrometers looking into the same interaction region, to record the photoelectrons. The technique, which was deployed at the European XFEL for the first time, substantially increased the achievable energy resolution and accuracy compared to previous studies (Figure 1).

Helml, Ilchen, and their colleagues are pleased with the outcome of the characterization study. "We were able to measure not only the first isolated attosecond pulses at the European XFEL, but also pulses possessing two spikes that we can sort according to their delay in time", says Ilchen. "We thus opened the door to pump–probe experiments, where we can initiate distinct processes with atomic precision with the first spike and directly interrogate the system with the subsequent spike."

Michael Meyer, leading scientist at SQS, adds: "We found the different pulse shapes to be statistically connected with specific operation modes of the European FEL. This knowledge will help us to further develop the facility's capabilities to generate such attosecond X-ray pulses and enable us to move forward into an era of target-tailored attosecond experiments."

Figure 2 shows two of these characteristic operation modes with substantially different SASE pulse profiles. The goal is that scientists will eventually be able to use the method at SQS to extract all accessible pulse profile information online during their experiments, i.e. within a fraction of a second, and to correlate and adjust their data analysis accordingly.

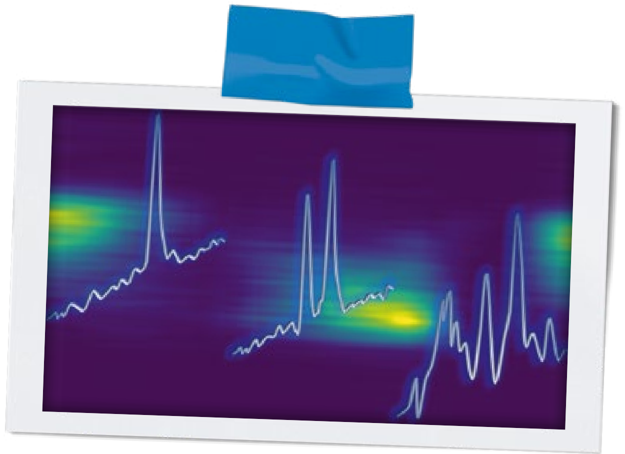


Figure 1:

Temporal structure of SASE pulses with sub-femtosecond resolution, reconstructed by angular streaking. From left to right: Isolated single-spike lasing event in the attosecond regime, dual-spike lasing event with a delay of about 2 fs between the two spikes, and multi-spike pulse of a few femtoseconds duration. The background shows a simulated detector image generated for training of machine-learning-based pulse characterization [1], depicting the detection angle vs. the flight time in the *x* and *y* direction, respectively.

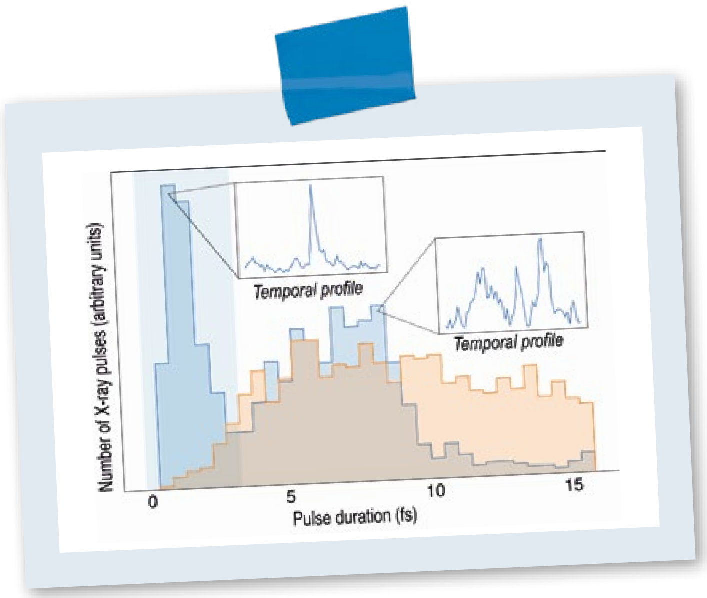


Figure 2:

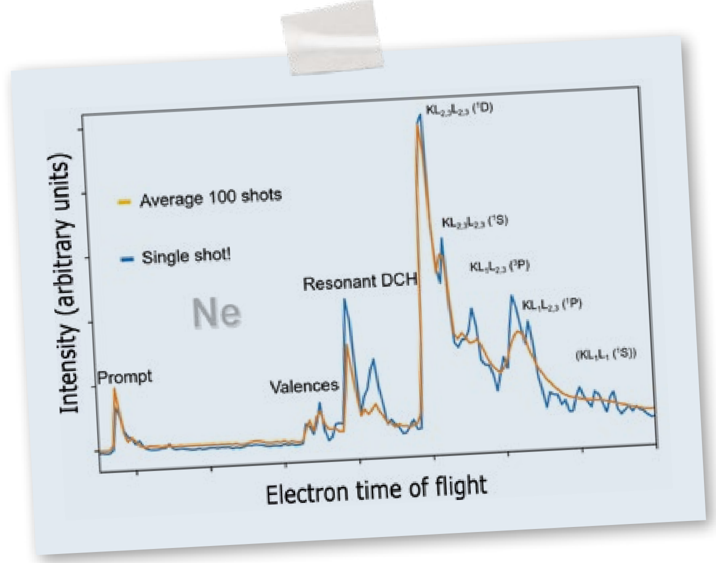
Comparison of two specific European XFEL operation modes during the attosecond campaign in 2022. One of the schemes (blue) led to an unprecedentedly significant production of attosecond pulses. The multi-spike operation is shown as a reference (red).

For their first attosecond time-resolved experiment, the scientists studied the electron restructuring of "hollow" neon after the ultrashort X-ray FEL pulse ejected both highly bound core electrons. The underlying processes in a highly transient system with a lifetime of only about 2 fs had been spectroscopically investigated for the first time in the first user experiment at SQS in 2018 [3]. "Now, these processes can be studied directly as they evolve in time, thanks to the special spectroscopy we used and the extremely high X-ray intensities provided by the European XFEL, which allowed us to measure these processes even in single shots", Helml reports.

Figure 3 illustrates some of these measurements. The resonant double-core hole (DCH) signatures can unprecedentedly be recorded in single shots—i.e. with individual X-ray pulses—using the new modes of attosecond operation and the special spectroscopy instrumentation. The combination opens the door to site-specific investigations of electron dynamics in matter, with interdisciplinary prospects for X-ray FEL research in general.

Figure 3:

Single-shot spectroscopy of neon Auger–Meitner spectra from single- and double-core holes (DCH) in comparison with a 100-shot average



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A JOURNEY TO THE CENTRE OF THE EARTH

Proof-of-concept experiment recreates conditions of deep Earth to investigate dynamics of planet interiors.

The lower mantle makes up over half of the Earth's total volume. Knowledge about the structure and composition of the lower mantle is important to understand more about planetary processes. However, recreating the extreme temperatures and pressures found in deep Earth is extremely difficult in the laboratory. In an experiment at the HED instrument, scientists used the unique parameters of the European XFEL to study the electronic spin state of iron and structural phase changes in the iron carbonate system. The proof-of-concept experiment opens the way for future studies of the chemistry and dynamics of planetary interiors.

If you were to take an elevator down to the centre of the Earth, you would first travel from the surface down through the Earth's crust, then through the subcontinental lithosphere, the upper mantle, and finally, some 600 km below the Earth's surface, you would reach the upper limit of the lower mantle. You would need to travel another 2300 km down through the lower mantle to finally reach the Earth's core; the lower mantle makes up over half the Earth's total volume. Conditions this far underground are extreme—temperatures in the lower mantle range from 1700˚C at its upper limit to around 3200 to 3700˚C at the border with the Earth's core; pressures range from 24 to 136 GPa.
For comparison, the pressure at the deepest point of our oceans, the Mariana Trench 11 km below sea level, is around 0.1 GPa.

The lower mantle is a crucial part of the Earth's complex structure. Convection currents in the lower mantle are understood to be important for driving tectonic plate movement; mantle plumes result in volcanic eruptions at the Earth's surface; and descending subduction slabs eventually make their way down to the lower mantle where they are recycled. The velocity and path of seismic waves, produced by and used as indicators of earthquakes, are significantly influenced by the composition of the lower mantle. And yet, due to the difficulties in sampling and studying materials under such extreme conditions, there is still no clear understanding of the lower mantle's composition.

Electrons in metal compounds can take on different spin configurations, affecting their physical behaviour. The spin states of iron in iron-bearing compounds—such as oxides, silicates, and carbonates—present in the lower mantle are thought to switch from a high-spin state to a low-spin state under particular pressure and temperature regimes. The spin state of these compounds affects the mantle's physical properties—such as density, elasticity, and viscosity—information needed to conduct computational simulations of such properties.

"Determining how the extreme pressure and temperature regimes found in the lower mantle affect the spin state of iron-bearing compounds is crucial for our understanding of the chemical and physical properties and dynamics of our planet", says Ulf Zastrau, leading scientist at the HED instrument of the European XFEL.

It is not easy, however, to create these conditions in the lab. In a recent experiment at HED, a group of scientists, coordinated by researchers from TU Dortmund University in Germany, used the unique parameters of the European XFEL X-ray beam to heat and study iron carbonate samples at static pressure. With the extremely intense X-ray beam, delivered in rapid pulses, it was possible not only to heat a sample to extreme temperatures but to maintain the high temperature for the prolonged time frame of several minutes needed for the experiment, while the sample was pressurized using a so-called diamond anvil cell (DAC). Consisting of two opposing diamonds with a sample compressed between the tips, DACs enable scientists to exert extremely high pressures onto any given sample (Figure 1).

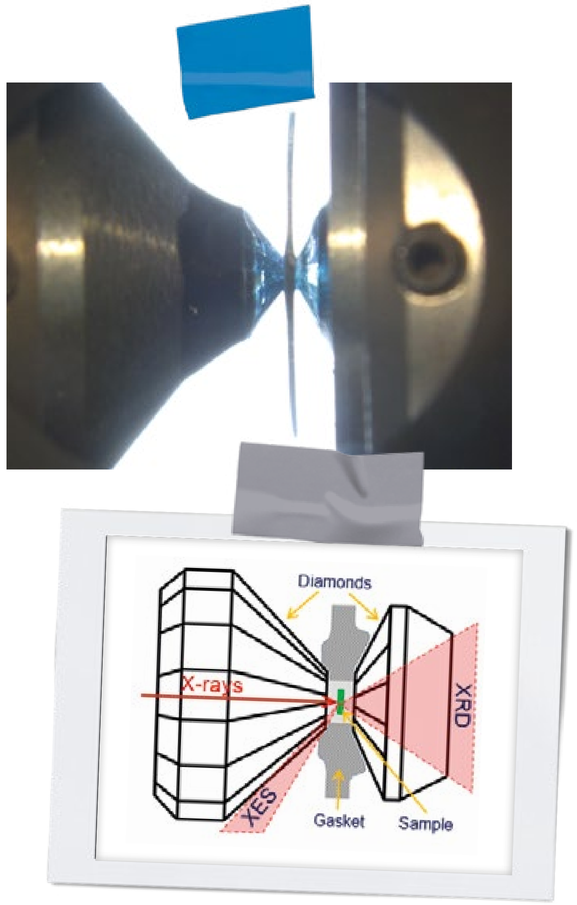

Figure 1:
Top: Photograph of a DAC. Bottom: Schematic of the DAC used at the HED instrument, with a 2.275 mm wide standard diamond upstream (left) and a 1.72 mm wide Boehler-Almax diamond downstream (right). The sample (green) is contained in a hole in a rhenium gasket with a diameter of 100 µm. (XES: X-ray emission spectroscopy, XRD: X-ray diffraction)

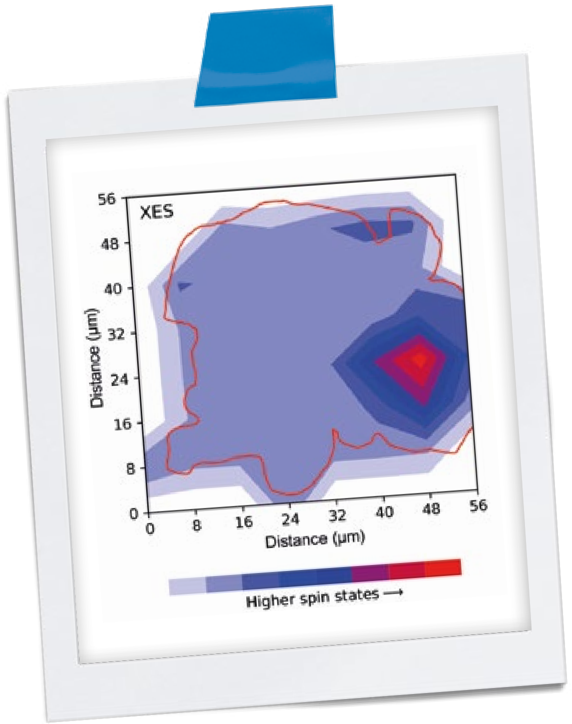

Figure 2:
The X-ray emission spectroscopy map shows the high-spin state (red) in the heated spot relative to the surrounding low-spin iron carbonate (blue). The sample's approximate outline is marked in red. Measurements were conducted while the sample was still under high pressure.

"Thanks to the unique combination of high pulse repetition rate, extremely brilliant X-ray beam, and the use of the DACs, we were able to create pressures of 51 GPa and reach melting temperatures in the iron carbonate samples", says Johannes Kaa from the TU Dortmund University team, who conducted the experiment with the HED group and researchers from Potsdam and Göttingen in Germany, Zürich in Switzerland, and Grenoble in France.

Initial data analysis indicates a complex process of change within the iron carbonate samples while under extreme temperature and pressure. Nonetheless, the scientists were able to gain insights into the spin state and structural changes of the samples. They observed that, during heating, first the volume of the low-spin iron carbonate increases dramatically when switching to high spin, then a more complex carbonate compound is formed, followed by melting with iron in the high-spin state.

The successful proof-of-concept experiment opens the way for more studies of the structure and dynamics of planet interiors. "With this type of experiment setup, we can increase our understanding of the Earth's interior and of other planets", says Kaa. "We now want to improve our approach for future experiments, where we hope to get even more detailed results at higher pressures and shorter time scales."

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EXCITING FLUORESCENT ELEMENTS

A new intensity correlation method demonstrates that X-ray fluorescence can be used for ultrafast imaging of materials.

If an atom absorbs light, such as X-ray photons, it can emit fluorescence light in return. Absorption of a photon creates an excited state of the atom that can then decay to the ground state through emission of a fluorescence photon characteristic of the element. The lifetime of the excited state is very short, typically 1 fs or less for a core electron excitation, so that, under usual illumination conditions, it is improbable to excite a large number of atoms in the specimen within this lifetime. The advent of X-ray FELs such as the European XFEL has changed that. At the European XFEL, the X-ray pulse used to excite the atom can be very intense and have a duration comparable to the lifetime of the excited state. Simultaneous excitation of an ensemble of atoms creates a collectively excited state, and intensity correlation maps of the fluorescence can then be used to produce images of the structure of the emitters, potentially down to atomic resolution. This method could mark a step forward toward the imaging of dense plasmas, macromolecules, or clusters of atoms.

Fluorescence is a well-known process that provides the basis for various structural characterization methods, such as X-ray fluorescence spectroscopy. Thanks to the ultrashort, high-intensity pulses of X-ray FELs, it is now possible to excite many atoms of the specimen within the lifetime of the excited state, which is on the order of 1 fs or shorter for K-shell excitation of heavy atoms by hard X-rays. This collective excitation means that many atoms decay simultaneously (within the excited state's lifetime). A spatial correlation analysis of the emitted fluorescence, together with application of a phase retrieval algorithm, can then be used to generate an image of the fluorescent atoms. This method—called "incoherent diffractive imaging" or "fluorescence intensity correlation imaging"—has, until now, been practically impossible because of low signals. The ultrashort and ultrabright X-ray beam generated by the European XFEL, combined with the megahertz repetition rate, makes this method applicable for the first time in imaging experiments at the facility's MID instrument.

"As we seek to explore the structure of a wider range of molecules and materials as well as dynamics that occur on unfathomable time scales, we need a greater range of tools and methods", says European XFEL leading scientist Anders Madsen. "Our extremely bright X-ray pulses arriving at megahertz repetition rate enable experimental techniques we could only dream about in the past."

A team of scientists has now successfully tested the new method at the MID instrument. For the proof-of-principle experiment, the team used copper foils to demonstrate that imaging by X-ray fluorescence intensity correlation can indeed provide an image of the fluorescing structure

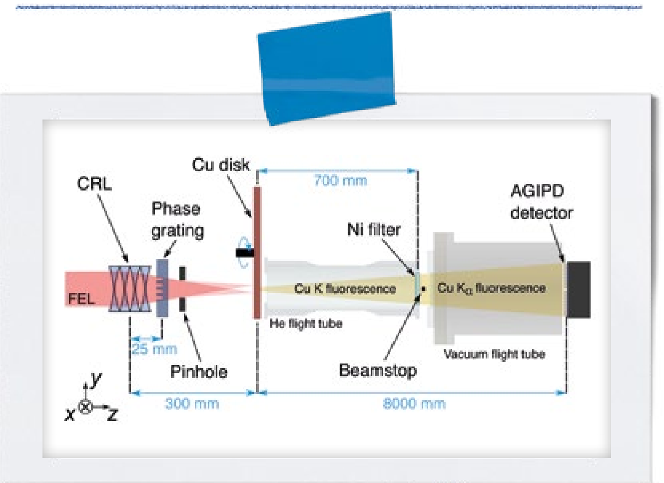

Figure 1: Sketch of the experiment setup (CRL: compound refractive lenses, Cu: copper, Ni: nickel, He: helium)

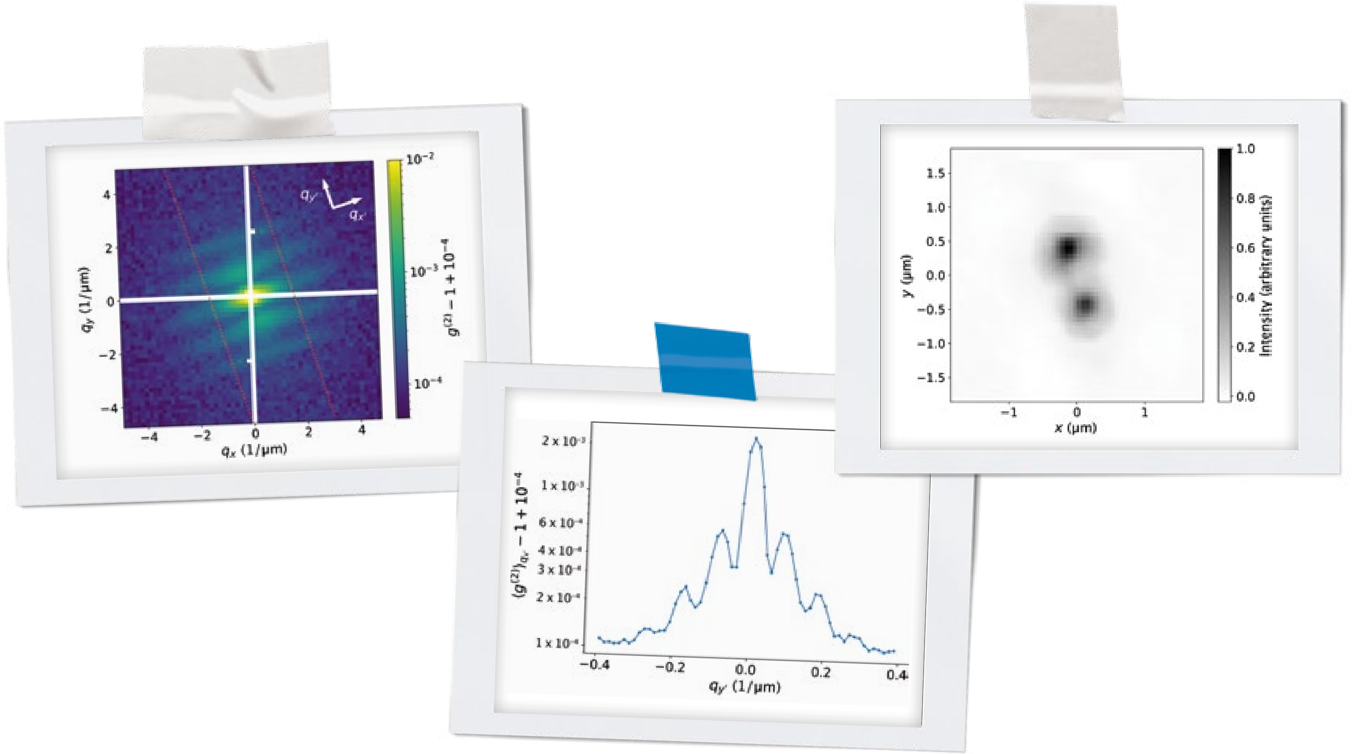

Figure 2: Left: Measured signal of the second-order correlation function $g^{(2)} - 1$ in logarithmic representation. Centre: Cut through the $g^{(2)} - 1$ signal along the direction of the grating modulation $q^{y'}$ and integrated along $q^{x'}$. The oscillatory behaviour evidences the structured illumination (two beams) of the copper disc due to phase modulation by the grating (see Figure 1). Right: Reconstructed fluorescence emitter distribution at the copper disc with the two beam spots clearly visible.

(Figure 1). A copper foil was excited by a series of highly focused X-ray femtosecond pulses. Because each pulse was intense enough to damage the foil, the foil had to be moved between pulses to ensure that the X-ray beam hit a different area each time. The time gap between pulses was 444 ns, so the foil had to move at a speed of over 30 m/s between the pulses. To achieve this rapid movement, the foil was mounted on a spinning disc. After the foil absorbed the X-ray energy, the generated fluorescence photons were picked up by a detector several metres away. The detector recorded separate images for every exciting pulse, fully exploiting the megahertz repetition rate of the European XFEL. By correlating where the emitted photons were hitting the detector within one exposure, an image of the fluorescing structure could be pieced together (Figure 2).

"This approach has promise for a range of different experimental scenarios", says Fabian Trost from DESY, who led the study. "In the future, it might be possible to obtain high-resolution three-dimensional images of fluorescing structures for real-time analyses, for instance of the formation and evolution of dense plasmas, which are relevant for fusion energy research."

Furthermore, the team says the method could be used in combination with other X-ray imaging techniques, complementing other datasets and analyses and possibly even enabling imaging of macromolecules or clusters. "For the first time", concludes Madsen, "it was shown that quantitative imaging by X-ray fluorescence intensity correlation is a feasible method for studying the structure and dynamics of matter at the European XFEL."

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MAGNETIC INSIGHTS

X-ray absorption spectroscopy experiments reveal details of fundamental mechanisms of magnetism.

Although magnets are familiar to us all, details of the underlying mechanisms of magnetism are still largely unknown because of the challenges involved in studying ultrafast processes that occur across minute distances. At the SCS instrument, researchers have used new approaches to study these mechanisms in two recent experiments. A better understanding of magnetism could inform the development of faster and more efficient data storage technologies.

From the simple fridge magnet to computers and enormous medical imaging devices, magnets are integral parts of our material world. These familiar objects exhibit a type of magnetism called "ferromagnetism", which occurs on its own without an external magnetic or electric field. Only a few substances exhibit these unusual properties—most commonly iron, nickel, and cobalt as well as their alloys.

"Humans have known about magnetism for millennia", says European XFEL Scientific Director Serguei Molodtsov, "and yet we still lack a truly comprehensive picture of the underlying electronic and atomic structure and dynamics that cause this familiar phenomenon."

Magnetism is the result of the interplay of atomic processes. A crucial factor is the spin direction of the electrons that surround the atom cores in the metal or metal alloy. Electrons can spin in one of two directions, either "up" or "down", creating a mini magnetic field as they do so. In ferromagnetic materials, all electrons spin in the same direction, generating a magnetic field across the entire metal. However, spin alignment occurs only when the electron shells are not completely filled. When nearby atoms have unequal numbers of electrons in their shells, the difference in charge means that they repel each other, forcing the electrons to align their spin direction. This is known as exchange interaction. The interplay between this interaction, how the effect dissipates across the material, and the forces that build up between electrons is what drives and influences the ferromagnetism in the material.

"With the unique parameters of the X-ray beam generated by the European XFEL, we now have the possibility to explore the dynamics and structures of ultrafast processes, such as magnetism", says Molodtsov.

Two recent experiments at the SCS instrument made use of these unique capabilities to study electron dynamics in nickel.

"Before we can address magnetic dynamics, we need to understand how to use the X-ray beam properly and what happens if we do not pay attention", says Martin Beye from DESY, who led the first project at SCS [1]. In this study, which used an approach called "non-linear X-ray absorption spectroscopy", the intensity of the X-ray beam was continuously increased until the scientists managed to evaporate the sample in just a single shot. The researchers then continued to increase the intensity even beyond that point. With careful analysis and simulations, they were able to establish the destruction mechanism and understand the effect this had on the measured data. "Based on our study, we have formulated a recipe on how to properly perform these types of experiments—information that has already been used for subsequent studies on magnetism", says Beye.

This information was extremely valuable for Andrea Eschenlohr from the University of Duisburg-Essen and her collaborators when they set out to design their experiment, which studied electron dynamics in nickel.

"A better understanding of how magnetism works in different metals could help inform the development of, for example, much needed improved data storage solutions with increased storage capacity and writing speed", explains Eschenlohr. "Changing magnetism with ultrashort laser pulses could be one concept for such future devices, but, in order to realize this approach, it is necessary to understand exactly how the electrons and their spins move after the laser pulse hits the ferromagnetic material."

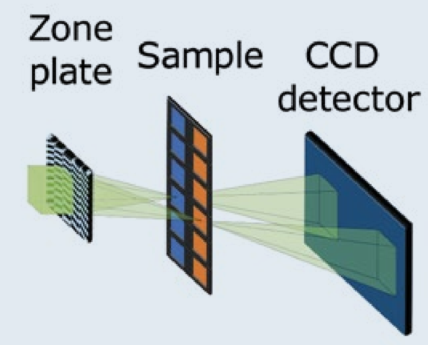
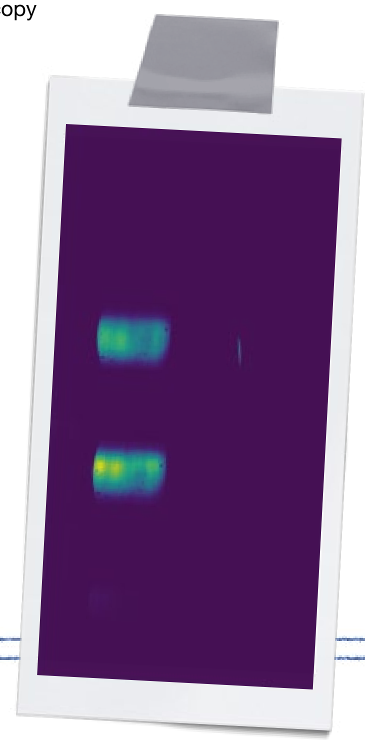


Figure 1: X-ray absorption spectroscopy at the SCS instrument uses a special zone plate, which generates two adjacent beam foci for transmission through the sample and a reference membrane before the beams impinge on the CCD detector.

Figure 2: Raw experimental data observed through nickel sheets as seen by the CCD detector in X-ray absorption spectroscopy



In their experiment, the researchers used a method called "time-resolved X-ray absorption spectroscopy" (Figure 1). First, a laser was used to initiate a magnetic change in the nickel samples, prepared as thin sheets mounted in the path of the X-ray beam. Then, the induced changes were recorded with the help of a series of extremely fast X-ray pulses delivered in quick succession—fast enough that the details of the ultrafast processes could be observed. The data was recorded using a charge-coupled device (CCD) detector (Figure 2), and the resulting series of snapshots revealed in detail how the electrons were reorganized following the initial laser impulse and how the electronic structure of the ferromagnetic metal changed on these ultrashort time scales [2].

The scientists are excited about these first results, which were achieved using specialized X-ray optics set up at the SCS instrument that enabled them to collect data of the high quality needed to recognize such details [3]. "By using ultrafast time resolution soft X-ray absorption spectroscopy, made possible by the unique capabilities of the European XFEL, together with computer modelling, we can access details of the electronic structure of magnetic materials", says Tobias Lojewski from the University of Duisburg-Essen, the Ph.D. student who performed the data analysis.

The scientists are now working towards refining the setup and approach for future experiments.

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INSTALLATION OF SOFT X-RAY PORT COMPLETE

New instrument expands European XFEL experiment portfolio.

The installation of a new instrument, called the Soft X-Ray Port (SXP), at the European XFEL was completed in 2022, raising the number of instruments using soft X-rays to three and the total number of instruments to seven. Commissioning of SXP has begun, and first users will arrive in summer 2023. The instrument allows users to bring their own experiment setups and is expected to help researchers understand the fundamental science relevant to numerous fields, from materials science to climate change.

In 2022, a third instrument on the SASE3 beamline was successfully installed, including completion of the technical infrastructure and beginning of the instrument's commissioning. Despite setbacks caused by the COVID-19 pandemic, the SXP instrument (Figure 1) was completed with only a few months delay and within budget.

"This was a huge undertaking, involving many groups across European XFEL and beyond", says Gerd Wellenreuther, head of the Project Management Office. "We look forward to completing commissioning and performing first user experiments", adds SXP group leader Manuel Izquierdo.

SXP is one of three instruments using soft X-rays with wavelengths of 0.4–4.7 nm, about 100 times shorter than the wavelengths of visible light. SXP provides the flexibility to accommodate different experimental instrumentation by allowing users to bring their own experiment stations. This offers the opportunity to try out new experimental techniques beyond the portfolio currently available at the European XFEL's other two soft X-ray instruments, SCS and SQS. Likewise, SXP can be used as a test bed for new, emerging techniques. Basic research at SXP will help address grand challenges. For example, studies of catalysts, new batteries, and light-harvesting materials can contribute to developing environmentally friendly energy production pathways.

The first new class of experiments performed at SXP involves time-resolved X-ray photoelectron spectroscopy (TR-XPES) on solids. An international community of scientists working on TR-XPES came together to form the TR-XPES User Consortium, involving DESY and the universities of Hamburg and Mainz and currently led by Kiel University. This consortium has contributed to the SXP project.

Construction of SXP's hutches and infrastructure began in 2020 and was completed in 2022. Six development projects were defined to ensure timely and coordinated implementation. Each of the six projects focused on a distinct element of the installation, such as the beamline components, the vacuum system, the laser system, and, as a first experiment station, a photoemission apparatus. This involved the entire Data Department, alongside most of the Instrumentation Department.

At the beginning of August 2022, the first X-ray beam was delivered to the SXP experiment hutch (Figure 2), and radiation protection tests could be performed. Radiation protection personnel interlock and safety equipment protection systems were installed by the radiation protection teams from both European XFEL and DESY. The X-ray beam was then transported sequentially to the

Figure 1: SXP instrument setup after official commissioning

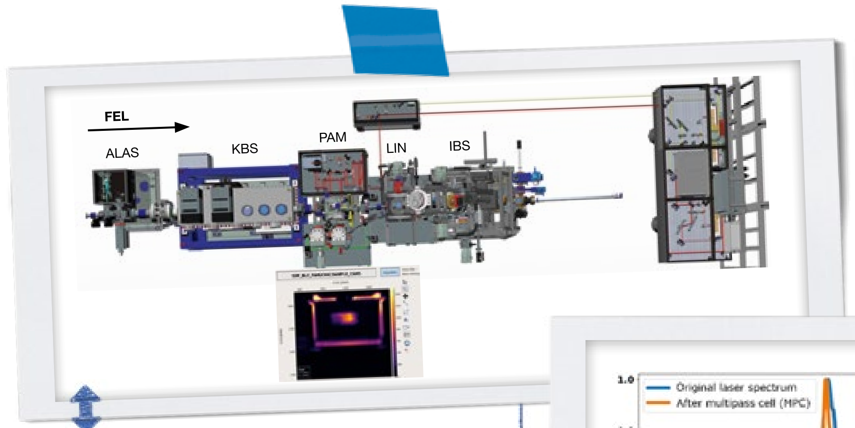


Figure 2: The SXP instrument and its permanent beamline components, including an inset showing the monochromatic X-ray beam at the pulse arrival monitor. This corresponds to the high photon energy configuration of the SASE3 beam transport system. (ALAS: alignment laser, KBS: Kirkpatrick–Baez focusing system, PAM: pulse arrival monitor, LIN: laser in-coupling, IBS: instrument beam stop)

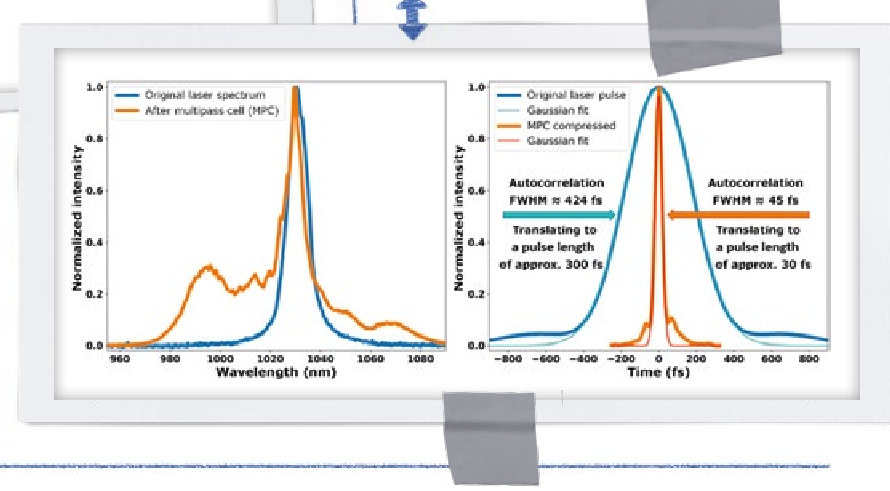


Figure 3: Left: Typical laser spectra before and after passing a Herriott multipass cell. Right: Autocorrelation measurements of the original and compressed laser pulses showing a reduction in pulse lengths from 300 fs to about 30 fs.

beamline's permanent components: an alignment laser, a pulse arrival monitor, and a laser in-coupling unit, all held in a dedicated vacuum system.

"The X-ray beam entering the instrument for the first time was an important milestone", says Izquierdo. "It required the collaboration of many groups. One of the most significant aspects of the project involved the Data Department, which had to connect and bring to life all parts of the instrument within the European XFEL control system." The Data Department had to link all electronic parts of the instrument with a data system, so future experiments could be seamlessly controlled. A full integration into central control and data management systems will be done in April 2023.

Another key part of SXP is the laser system. A pump–probe laser can be used to excite samples before they are studied with the X-ray laser. "With the pump–probe laser, we provide a large range of wavelengths from 200 nm to 10 µm, offering users a great deal of flexibility," says Patrik Grychtol, laser specialist of the SXP group. In addition to the pump–probe laser, an independent laser is available (Figure 3), providing a pulse duration of 200 fs that can be reduced to 45 fs. The team plans to extend the available spectrum of photon energies into the ultraviolet range in the future. The pump–probe laser will be commissioned in March 2023.

The commissioning of the SXP instrument was officially started in October 2022. "Planning, construction, and commissioning of the SXP instrument are the result of many years of joint effort by European XFEL and several research groups of the TR-XPES User Consortium", says European XFEL Scientific Director Serguei Molodtsov. "We look forward to welcoming the first users in 2023."

The TR-XPS setup at the SXP instrument provided by the TR-XPS User Consortium is equipped with a momentum microscope photoelectron spectrometer. This spectrometer was put under vacuum just before the end of 2022. User experiments involving TR-XPS, due to start in 2023, will provide an advanced understanding of the electronic, magnetic, chemical, and atomic structure properties of solid materials, thanks to the femtosecond time resolution of SXP.

"The new instrument will help us to address grand challenges targeted by European XFEL, such as investigating new environmentally friendly energy pathways or better understanding the atmospheric processes that influence climate change", concludes Izquierdo.

This project has been enabled by the contributions of the following groups:

Controls, Data Analysis, Detectors, Electronic & Electrical Engineering, Hall Crew, IT & Data Management, Lasers, Mechanical Engineering, Procurement, Project Management Office, Safety and Radiation Protection (European XFEL and DESY), SXP, Technical Services, Vacuum, X-Ray Operations, X-Ray Optics, X-Ray Photon Diagnostics

External contributors
TR-XPS User Consortium, Kiel University, Universität Hamburg, Johannes Gutenberg University Mainz, DESY

NEW LASER FOR CREATING MATTER WITH HIGH ENERGY DENSITY NOW ONLINE

The DiPOLE-100X laser system is ready for user experiments at the HED instrument in 2023.

A new laser system that will be used to generate high energy density states in matter went into operation at the HED instrument in 2022. The DiPOLE-100X laser system is an in-kind contribution from the HiBEF User Consortium. It can deliver infrared laser pulses of arbitrary temporal shapes from 500 ps to 20 ns with pulse energies up to 100 J at a wavelength of 1030 nm and repetition rates up to 10 Hz. With its pulse-shaping capabilities, the DiPOLE-100X can be used to achieve a wide range of pressure–temperature conditions to enable studies of planetary interiors.

The high-repetition-rate, high-energy DiPOLE 100-X laser was developed exclusively for the European XFEL at the Science and Technology Facilities Council (STFC) Central Laser Facility in the UK as an in-kind contribution by STFC, UK Research and Innovation (UKRI), the University of Oxford, and the Engineering and Physical Sciences Research Council (EPSRC) within the HiBEF User Consortium. By June 2022, the laser had been reconstructed in its new home and commissioned to the desired energy output.

“We are very excited to see the DiPOLE laser now installed at the European XFEL”, says Ulf Zastrau, leading scientist at the HED instrument. “In combination with other beamline components, it will be used to generate extreme temperatures and pressures similar to the interior of far-off planets, enabling us to do diffraction and spectroscopy experiments to help us better understand the geology of these exoplanets.”

With the DiPOLE-100X laser, scientists will be able to create temperatures of up to 20 000°C and pressures of up to 3 000 t/cm². The atomic structure and dynamics of these extreme states of materials can then be studied using the ultrabright and intense X-ray pulses produced by the European XFEL.

The unique laser is extremely versatile, producing infrared pulses of arbitrary shapes from 500 ps to 20 ns with pulse energies up to 100 J at a wavelength of 1030 nm and repetition rates up to 10 Hz. The pulse-shaping capabilities of the DiPOLE-100X make it possible to achieve various pressure–temperature conditions in materials using techniques such as single shocks, multiple shocks, ramp compression, or any combination thereof. “With this setup, we will be able to study processes such as phase transition dynamics, plastic deformation, spallation, or high-speed plasma flows”, explains Zastrau.

The DiPOLE-100X is used to irradiate samples in HED Interaction Chamber 2, a target chamber for X-ray diffraction. Other important developments in 2022 included the installation of the beam transport system from the laser hutch to the interaction chamber; this was achieved in summer 2022, along with the recommissioning of the DiPOLE-100X laser system. The beam transport also comprised a laser frequency doubling system that converts infrared light (1030 nm wavelength) to green light (515 nm), which is advantageous for laser–matter interaction. The first frequency-doubled light was generated in September 2022.

For the characterization of laser-compressed matter, a velocity interferometer system for any reflector (VISAR) diagnostic system was developed. “The VISAR provides us with comprehensive information about the sample conditions, which is vital for our experiments”, says Zastrau. The VISAR also requires a low-energy probe laser. As no

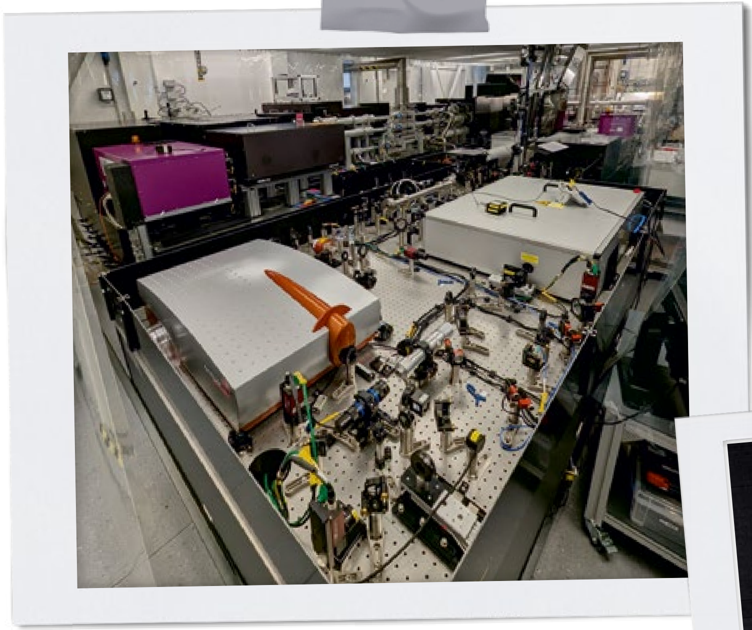


Figure 1:

View of the DiPOLE-100 X, a kilowatt-level, diode-pumped, solid-state laser

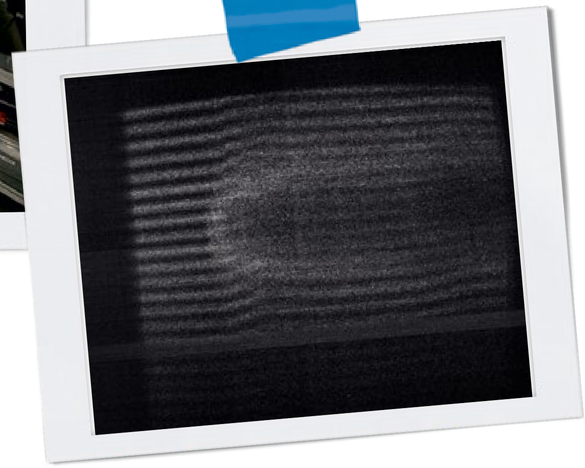


Figure 2:

First shock generated with the DiPOLE-100X laser in HED Interaction Chamber 2, registered with the VISAR system

system with the specifications required for the European XFEL was available on the market, the laser was developed in-house, together with Laboratoire pour l’Utilisation des Lasers Intenses (LULI) in France. The installation of the VISAR system started in spring 2021 and was completed at the end of the year. The VISAR laser can measure velocities of reflecting surfaces ranging from less than 100 m/s to more than 50 km/s with a temporal resolution better than 50 ps. The three VISAR arms enable a wide range of detectable velocities in a single experiment and reflectivity at two different wavelengths.

Together, the DiPOLE-100X laser and the VISAR make up a platform for direct laser compression experiments. At the end of 2022, the complete platform was tested by irradiating aluminium with a laser energy of 30 J at a frequency-doubled wavelength of 515 nm. The resulting shock breakout was detected successfully with the VISAR system (Figure 1).

“This experiment represented the final test of the complete system”, explains Zastrau. “We demonstrated the performance of all the subcomponents—laser, beam transport, and VISAR systems—and are now looking forward to using the platform for the first user experiments with X-rays.”

A community experiment with over 80 contributors is scheduled for May 2023. Its aim will be first to jointly check the setup with reference systems and then to study phase transitions, elastic properties, melting, and liquid structure of iron, iron–silicon alloys, and carbon polymorphs. The experiment will use an X-ray diffraction approach with high laser energies and unprecedented repetition rate and cover a unique range of experimental conditions.

This contribution was enabled by the work of the HED and HIBEF groups at European XFEL and the STFC team.

NEWS AND EVENTS

First X-ray FEL beam at the SXP instrument

NEWS AND EVENTS

24 January

Felix Büttner wins Walter Schottky Prize

The Walter Schottky Prize of the German Physical Society (DPG) honours outstanding work by young physicists in solid-state research. The 2022 award went to physicist Felix Büttner from Helmholtz-Zentrum Berlin for his insights into magnetic skyrmions, which he developed at the European XFEL.

Felix Büttner, Helmholtz-Zentrum Berlin

26 January

Users' Meeting with scientists from more than 40 countries

In 2022, for the second time in a row, the European XFEL Users' Meeting was held as a virtual meeting. It took place in parallel with the DESY Photon Science Users' Meeting, with over 2000 scientists from 40 countries attending the event.

FXE instrument at the European XFEL

27 January

Young Scientist Award for Camila Bacellar

Camila Bacellar was honoured with the European XFEL Young Scientist Award for her research on heme proteins using femtosecond X-ray spectroscopy at the FXE instrument. Bacellar is a beamline scientist at the SwissFEL at PSI in Switzerland.

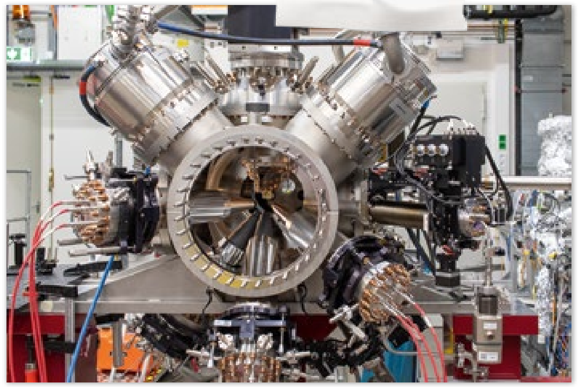
Camila Bacellar, European XFEL

13 February

Racing against one of the fastest atomic processes

Auger–Meitner decay is one of the fastest relaxation processes involving X-rays, occurring within a few millionths of a billionth of a second. A team of scientists led by the University of Connecticut, USA, and CFEL in Hamburg discovered a new process at the European XFEL's SQS instrument that is at least as fast as Auger–Meitner decay. The research demonstrates how X-ray FELs can be used to measure ultrafast processes.

Physical Review Letters (doi:10.1103/PhysRevLett.127.213202)



Atomic-like Quantum Systems (AQS) experiment station at the SQS instrument, which was used for the experiment

16 February

3D printing enables customised sample delivery

A prerequisite for experiments at the European XFEL is the precise delivery of samples into the X-ray beam, tailored to the corresponding experiment. The Sample Environment and Characterization (SEC) group developed various devices for liquid sample injection that can be produced in large numbers by means of 3D printing.

Journal of Synchrotron Radiation (doi:10.1107/S1600577521013370)

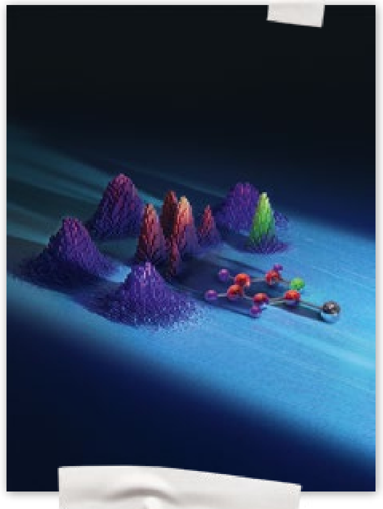
European XFEL scientist Mohammad Vakili testing a nozzle

21 February

Molecule snapshot by explosion

Exploding a molecule to take its picture? A research team led by European XFEL and CFEL used the X-ray flashes generated by the European XFEL to take snapshots of gas-phase iodopyridine molecules at atomic resolution. The X-ray laser caused the molecules to explode, and the image was reconstructed from the pieces. The results are an important step towards recording molecular movies.

Nature Physics (doi:10.1038/s41567-022-01507-0)



The fragmentation pattern (left) enables scientists to infer detailed information on single molecules (right).

3 March

Australia awards CSIRO Alumni Scholarship

Trey Guest, a Ph.D. candidate at the La Trobe Institute for Molecular Science (LIMS), was awarded the 2022 CSIRO Alumni Scholarship in Physics for research at the European XFEL. As Australia's national science agency, CSIRO awards the physics scholarship to help connect the country's brightest young physicists and mathematicians to leading research centres around the world.

Trey Guest, La Trobe University, Australia

24 March

Statement on the war in Ukraine published

Management and staff of European XFEL published a statement on the War in Ukraine, endorsed by the shareholders representing Denmark, France, Germany, Hungary, Italy, Poland, Slovakia, Spain, Sweden, Switzerland, and the United Kingdom.

European XFEL staff members hold a moment of silence to remember the innocent victims of the war and express their solidarity with the people of Ukraine.

25 March

Topping-out ceremony for new office building

European XFEL held a topping-out ceremony for a new office complex on its research campus in Schenefeld. The building provides workspaces for 184 employees in 56 offices totalling around 3000 square metres. Construction started at the beginning of August 2021. The costs of the office complex will amount to around 8.2 million euro.

European XFEL Managing Director Nicole Elleuche at the topping-out ceremony

28 March

Virtual SRI conference attended by over 1160 participants

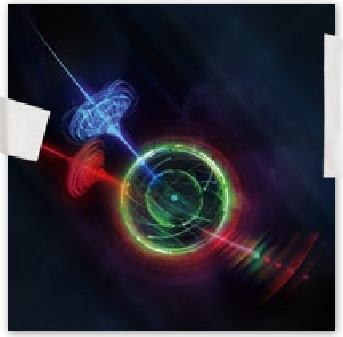
The 14th International Conference on Synchrotron Radiation Instrumentation (SRI2021) was organized as a virtual meeting by DESY and European XFEL in 2022. It was attended remotely by more than 1160 scientists from around the world. The SRI conference is one of the largest exchange forums in this field, where the latest developments in technologies, instrumentation, and research are discussed.

11 April

Record time resolution

In an experiment at the European XFEL's SQS instrument, a team from European XFEL and DESY demonstrated a record time resolution of around 15 fs—the best resolution reported so far in a pump–probe experiment at an X-ray FEL, while keeping a high spectral resolution. The results enable the observation of ultrafast processes in materials that were not accessible before.

Optica (doi:10.1364/optica.454920)

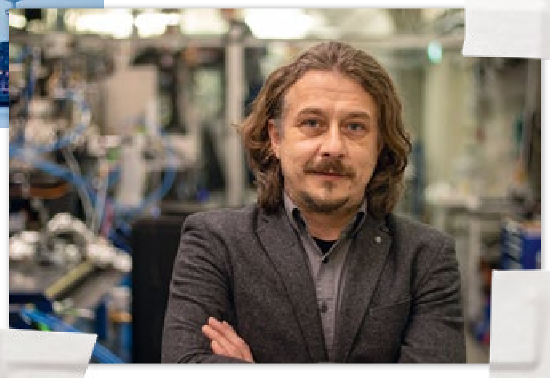


An ultrashort X-ray pulse and an optical laser pulse interact simultaneously with a neon atom.

21 April

EIC Pathfinder grant awarded to Patrik Vagovic

Patrik Vagovic, a scientist from the SPB/SFX instrument at the European XFEL and CFEL at DESY, was awarded one of the first European Innovation Council (EIC) Pathfinder grants. As part of the grant, European XFEL receives 813 750 euro across a three-and-a-half-year period. Vagovic is constructing an X-ray microscope prototype that will be able to image samples from different angles using individual European XFEL X-ray pulses, providing insights relevant to the life sciences as well as the aeronautics and automobile industries.



Patrik Vagovic

22 June

European XFEL support for Ukrainian refugees

European XFEL and its staff organized support for people seeking refuge from the war in Ukraine. The European XFEL guest house opened its doors to refugees in early March and accommodated Ukrainian adults and children. European XFEL employees also set up an onsite collection point for donations to the Hamburg charity group Hanseatic Help.

Guest house at European XFEL

29 June

European XFEL signs Charta of Diversity

European XFEL signed the Charta of Diversity, joining over 4500 German organizations and institutions in pledging to create and sustain a workplace valuing all employees regardless of their age, ethnic origin and nationality, gender and gender identity, physical and mental abilities, religion and world view, sexual orientation, or social origin. The Charta of Diversity is an employer initiative under the current patronage of German Chancellor Olaf Scholz to promote diversity in companies and institutions.

Robert Feidenhans'l and Nicole Elleuche sign the Charta of Diversity at European XFEL.

4 July

Federico Boscherini new Chair of European XFEL Council

Federico Boscherini, Professor of Physics at the University of Bologna in Italy, took over as the new Chair of the European XFEL Council. With many years of experience in research with X-rays, Boscherini has been an advisor to the Council since 2018. James Naismith, Professor of Structural Biology at the University of Oxford, UK, became the new Vice Chair of the Council.

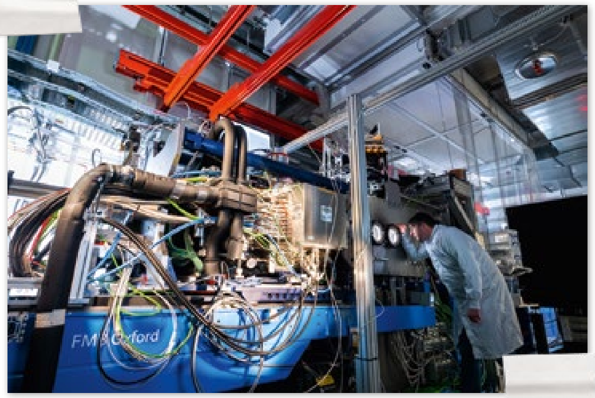
European XFEL Managing Directors Nicole Elleuche (left) and Robert Feidenhans'l (right) welcome Federico Boscherini (centre left) and James Naismith (centre right) to their new roles.

26 August

New method to unveil biological processes

A team of scientists involving European XFEL developed a new method for tracking the reactions of proteins. Called multi-hit serial femtosecond crystallography (SFX), it is particularly useful for studying molecules undergoing irreversible processes, which cannot be measured using synchrotrons or lab-based X-ray sources. The method, which was developed by La Trobe University researchers, allows scientists to monitor the reactions of proteins as they move, on sub-microsecond time scales.

Nature Communications (doi:10.1038/s41467-022-32434-6)



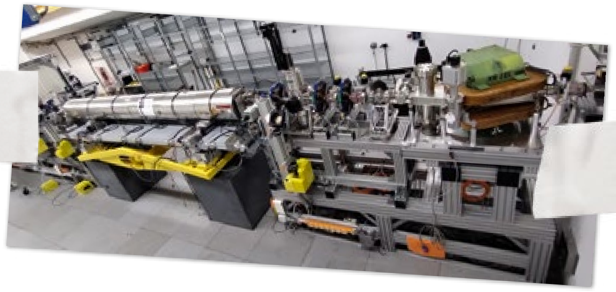
The SPB/SFX instrument is used to investigate crystalline and non-crystalline matter.

2 September

First light of a new laser

A new laser developed at the photoinjector test facility at DESY in Zeuthen (PITZ) and partly funded by European XFEL generated its first light. The new laser is also an FEL, but it produces radiation in the terahertz range, with much longer wavelengths compared to the European XFEL's short-wavelength X-rays. Together, the unequal siblings could provide new insights into the behaviour of electrons and magnetic fields in matter.

Proc. SPIE 8778, Advances in X-ray Free-Electron Lasers II: Instrumentation (doi:10.1117/12.2017014)

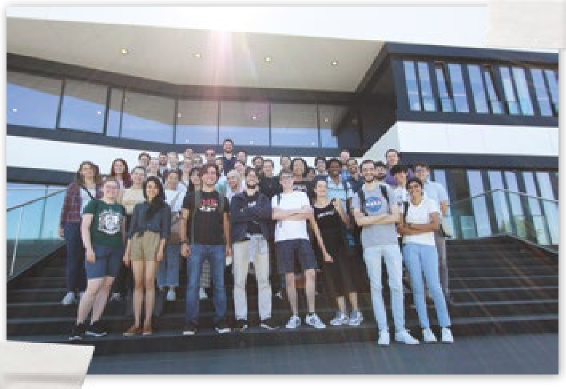


PITZ facility at DESY with the new terahertz FEL

16 September

Guided tours re-open to hundreds of visitors

European XFEL welcomed groups of visitors for guided tours on its research campus again starting in March 2022, after being closed to onsite visitors during the COVID-19 pandemic. Around 600 visitors took part in 40 guided tours of the facility between March and September. They included university students, high school classes, scientists, and representatives from politics and business.



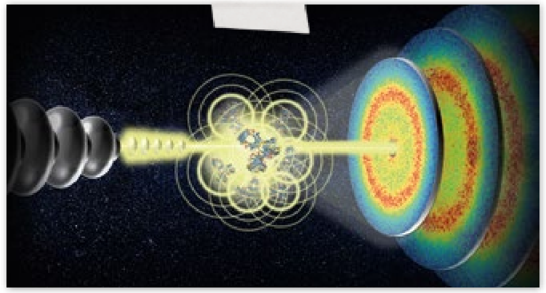
Participants of the DESY Summer Student Programme 2022 at European XFEL

23 September

Probing proteins in cell-like environments

A research team identified a new way of probing protein dynamics using the high repetition rate and coherence of the X-ray flashes produced by the European XFEL. The study, which relied on a technique called megahertz X-ray photon correlation spectroscopy (MHz-XPCS), could open new applications in health and pharmaceuticals. It was led by Stockholm University in Sweden, the University of Tübingen, the University of Siegen, and European XFEL in Germany and used the MID instrument to examine antibody protein solutions.

Nature Communications (doi:10.1038/s41467-022-33154-7)



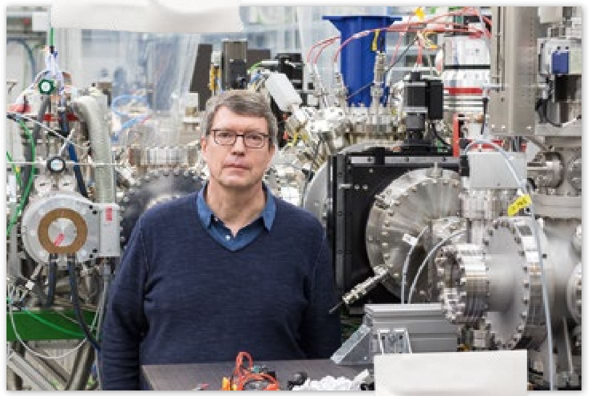
Artist's impression of the MHz-XPCS technique being used to measure the dynamics of proteins in dense solutions

26 September

Atom–photon process studied with extreme ultraviolet light

A collaboration involving European XFEL observed a phenomenon known as Rabi oscillations using extreme ultraviolet (XUV) light for the first time. Rabi oscillations—a quantum-mechanical process that occurs when intense light interacts with matter—underpin many applications in photonics and nanoelectronics. The results were part of a study led by Institut Lumière Matière, CNRS, in Lyon, France, that used the XUV pulses from the FERMI FEL in Trieste, Italy.

Nature (doi:10.1038/s41586-022-04948-y)



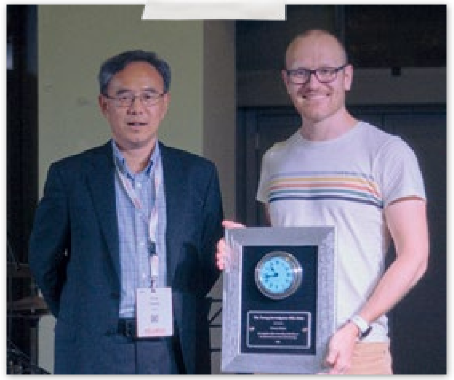
Michael Meyer, co-author of the study, at the European XFEL's SQS instrument

28 September

European XFEL scientists awarded Young Investigator FEL Prize

Two physicists at European XFEL, Jiawei Yan and Svitozar Serkez, were awarded the Young Investigator FEL Prize at the FEL2022 conference, held in Trieste, Italy. The award honours researchers under 35 years of age for achievements in FEL science. The two recipients, who are members of the FEL Physics group of European XFEL, received the prizes along with a third recipient, Zhen Zhang, from SLAC, USA.

Zhirong Huang (left) from SLAC, Chair of the prize committee, and prize recipient Jiawei Yan (right)



Zhirong Huang (left) and prize recipient Svitozar Serkez (right)

14 October

Science@FELS 2022 held at European XFEL

The Science@FELs 2022 conference was held at DESY and European XFEL in September with more than 100 participants from 12 countries in attendance. The conference, which is organized every two years by the FELs OF EUROPE collaboration, has evolved into one of the most important international meetings in FEL science. This year also marked the 10^{th} anniversary of FELs OF EUROPE. At the conference, the 2022 FEL Science and Applications prize was awarded to Praveen Maroju from the University of Freiburg, Germany.

Praveen Maroju being awarded the FEL Science and Applications prize by European XFEL Scientific Director Serguei Molodtsov, Chair of the Management Board of the FELs OF EUROPE Steering Committee

19 October

Industry collaboration reveals insights on drug targets

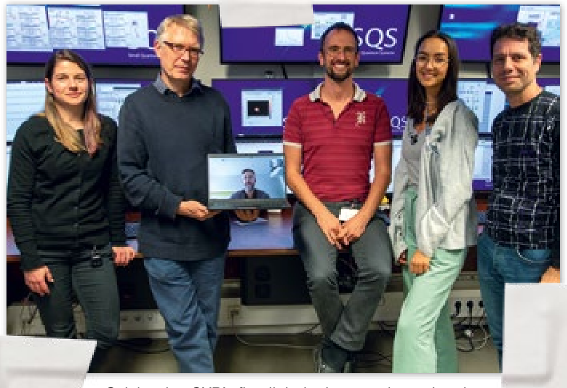
European XFEL conducted a pilot collaborative experiment with the international biopharmaceutical company Sosei Heptares. The experiment demonstrated a powerful approach to determining 3D structures of biomolecules with atomic resolution. The collaboration used the European XFEL's SPB/SFX instrument to investigate G protein-coupled receptor (GPCR) crystals (or StaR protein crystals) generated by Sosei Heptares. GPCRs are an important class of therapeutic drug targets, with around 30% of current marketed drugs targeting them.

European XFEL scientist Yoonhee Kim at the SPB/SFX instrument

20 October

First light at the new SXP instrument

The new Soft X-Ray Port (SXP) instrument at the European XFEL achieved its first X-ray light. SXP is designed to allow users to bring their own experiment setups and implement new techniques using the European XFEL beam. The third European XFEL instrument using soft X rays, it brings the total number of instruments at the facility up to seven.



Celebrating SXP's first light in the experiment hutch

25 October

European XFEL celebrates five years of user operation

European XFEL celebrated its fifth anniversary of user operation and launched the commissioning of its new SXP instrument in the presence of State Secretary Judith Pirscher from the German Federal Ministry of Education and Research (BMBF), Senator Katharina Fegebank from the Hamburg Authority for Science, Research, Equality and Districts, and around 150 guests and staff members.

Right: Hamburg Senator Katharina Fegebank and BMBF State Secretary Judith Pirscher start the commissioning of the SXP instrument.
Left: Wim Leemans (DESY) and Nicole Elleuche and Robert Feidenhans'l (both European XFEL) look on.

26 October

SIGN: A new network for Italian scientists in Germany

Scientists from European XFEL and DESY partnered with colleagues across Germany to form a new national network for Italian scientists, Scienziati Italiani in Germania Network (SIGN). The first network of its kind for Italian scientists working in Germany, it aims to support research and provide opportunities for knowledge transfer and professional networking. As one of the co-founders of the network, European XFEL Scientific Director Sakura Pascarelli signed its founding charter in Berlin in October.

Co-signatories at the official inauguration ceremony for SIGN

11 November

Celebration for Hamburg Prize for Theoretical Physics winner

European XFEL hosted a celebration for Nicola Spaldin, winner of the 2022 Hamburg Prize for Theoretical Physics sponsored by the Joachim Herz Foundation. Spaldin is a materials scientist and lecturer at ETH Zurich in Switzerland who is renowned for her theoretical prediction and later development of a new class of materials called multiferroics, which are also studied at European XFEL.

Nicola Spaldin (third person from left in the first row) during a visit to European XFEL.

23 November

Successful call for water research

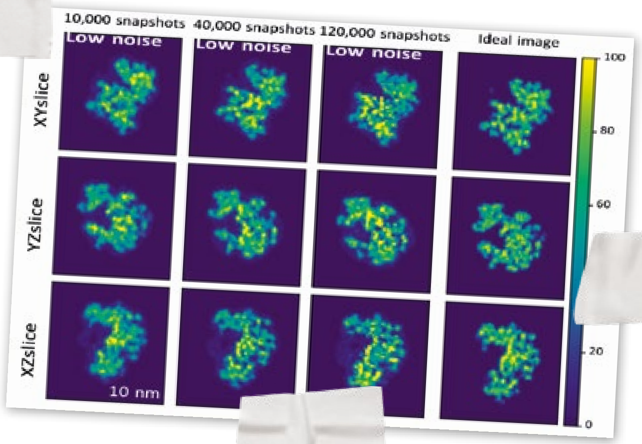
Water, a key to life on our planet, plays a central role in human cells, clouds in the atmosphere, water-based catalysts in industry, and many other important systems. In early 2022, European XFEL, together with DESY's Centre for Molecular Water Science (CMWS), launched a call for expressions of interest in water research with the goal of combining the unique X-ray infrastructure with international expertise in water-based science. A total of 25 proposals were submitted, with all six European XFEL instruments receiving requests for beamtime. Eight of these proposals were accepted for the first half of 2023.

8 December

New simulations enable faster biological insights

Single-particle X-ray diffraction imaging (SPI) is a technique used at the SPB/SFX instrument to study biological molecules in their native environments. By accurately simulating the SPB/SFX detector, researchers determined a route that could result in increased data collection efficiency and improved resolution of the images taken through SPI, enabling new insights into the structure and evolution of biological molecules.

Structural Dynamics (doi:10.1063/4.0000169)



Simulations of the structure of biological molecules for different numbers of image snapshots (panels on the left) compared with the "perfect" image (right)

MAGAZINE

Start of commissioning of the SXP instrument at our celebration of five years of user operation

FIVE YEARS OF USER OPERATION AT EUROPEAN XFEL

Figure 1:

BMBF State Secretary Judith Pirscher addresses the audience during the celebration.

In late September 2017, the first users arrived on the European XFEL Schenefeld campus. The first two instruments were available for use: FXE and SPB/SFX. But there was no BeamStop restaurant, no guest house, and, importantly, no onsite bee-keeping facilities (and, so, no *BeeTime* honey).

In the last five years, the company has developed rapidly. From the outset, the European XFEL was the most technologically advanced X-ray laser worldwide, with users from across the world taking advantage of the unique research opportunities. But the company now also has its own Ph.D. programme, currently with 45 students and over 450 hosted since operation began.

At the same time, European XFEL has expanded its technical and instrumental offerings. The facility now hosts six scientific instruments for users—including FXE, HED, MID, SCS, SPB/SFX, and SQS—with a seventh, SXP, whose commissioning began in 2022. Since operation started, the facility has received over 1060 research proposals, delivered over 16 300 hours of beamtime to over 4000 researchers, and produced 60 million terabytes of experiment data. Its performance has also grown annually from 1356 hours of beamtime in 2018 to 8000 hours in 2022, when it enabled over 100 user experiments.

The scientific instruments contribute to the facility's mission to address global challenges in climate and energy, digitalization, environment and sustainability, and health research. For example, European XFEL scientists are helping to develop a better understanding of the structural biology of antibiotic-resistant bacteria, potentially enabling pharmaceutical companies to produce more effective antibiotics. They are also conducting experiments on magnetic samples, uncovering new insights into data storage and stability. Some of European XFEL's research even takes us to distant gas giant planets, allowing scientists to probe the behaviour of matter under extreme conditions using specialized diamond-based chambers. European XFEL and DESY staff members also work continuously to further improve the quality of the X-ray beam and the performance of the instruments.

"We have grown rapidly both in terms of our capacity and in terms of our experimental capabilities in the last five years", says European XFEL Managing Director Robert Feidenhans'l. "We have been able to bring together more and more users to European XFEL, forming collaborations that allow us to target some of the biggest challenges we face in society, from health to the environment. We want to continue this successful development throughout the coming years."

"In a unique piece of teamwork of accelerator staff at DESY, beamline scientists at European XFEL, and users from around the globe—in combination with a robust technical design that was developed over almost 20 years—we were able to establish European XFEL very quickly as the world-leading X-ray FEL facility with an impressive scientific output", says Wim Leemans, Director of the Accelerator Division at DESY. "And we are far from the end in pushing the limits of this promising machine."

The facility and campus are also continuing to develop. The company built and opened its own restaurant, BeamStop, in 2019 and a guest house for visitors to campus in 2020. Since its opening, BeamStop has sold around 60 000 meals and around 47 000 cups of coffee. And the campus is continuing to grow, with a new office building due to open in 2023 and a new visitor and conference centre, Lighthouse, under construction for 2024.

A celebration to remember

On 25 October 2022, European XFEL celebrated its first five years of successful operation with State Secretary Judith Pirscher from the German Federal Ministry of Education and Research (BMBF) and Senator Katharina Fegebank from the Hamburg Authority for Science, Research, Equality and Districts, as well as around 150 guests and staff members (Figures 1 and 2).

Figure 2:

Ulf Zastrau, leading scientist at the HED instrument, playing the harpsichord at the event

State Secretary Pirscher said: "The European XFEL is a great success. The 850 million euro provided for its construction by the BMBF so far is a solid investment. With this, we are strengthening not only basic research but also the technological sovereignty of both Germany and Europe."

Three users engaged in an onsite panel discussion about their experiments and the reasons they enjoyed working at European XFEL.

The event was also the kick-off for the commissioning of the new SXP instrument (Figure 3). SXP is the third European XFEL instrument using soft X-rays, which have wavelengths between 0.4 and 4.7 nm, about one hundred times shorter than those of visible light. The SXP instrument will allow users to bring and temporarily establish their own experiment setups and to implement new techniques using the European XFEL beam. For more information on SXP, see the Technical Highlight on page 24.

Coming together as a community

In the five years since user operation began, the European XFEL community has had to deal with numerous challenges, the war in Ukraine and the COVID-19 pandemic being just two. But the collaboration and trust of the users, partners, staff members, and the entire European XFEL community has been one of the great strengths of the company.

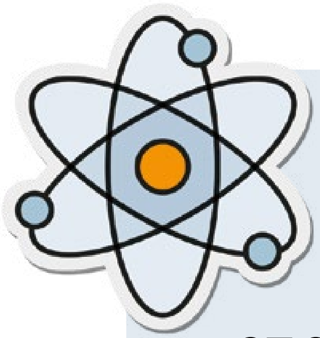
After having reached the milestone of five years of operation, the facility will continue to grow. Entering a phase of "harvesting"—in other words reaping the rewards of many years of ramping up operation—European XFEL will produce increasing and exciting experiment results and continue to further develop instrumentation and capabilities, enabling even more users to benefit from the unique facility. The company will also sharpen the strategic focus towards science that addresses society's biggest challenges: from climate and energy, to digitalization, to environment and sustainability, to health.

Figure 3:

Right: Hamburg Senator Katharina Fegebank and BMBF State Secretary Judith Pirscher start the commissioning of the SXP instrument.

Left: Wim Leemans (DESY), Nicole Elleuche and Robert Feidenhans'l (both European XFEL)

FACTSHEET



Electron and X-ray beams

27 000
Number of electron bunches per second

0.04 nm
Minimum wavelength of the X-ray flashes (30 keV)

10 µs
Time of flight of an electron from the injector to the dump (1/100 000 s)

32.9 W
Highest X-ray FEL beam power averaged over a second

3
Number of SASE undulators running in parallel

21 000
Highest number of X-ray flashes per second

ca. 50 µm
Diameter of the electron beam (comparable to the diameter of a human hair)

11 nm
Smallest focus of the X-ray beam

Users

95
User experiments

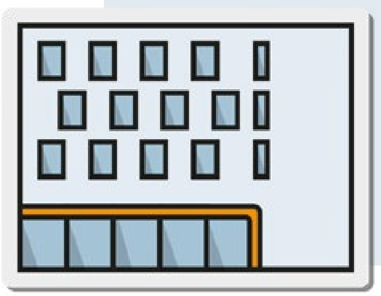
8080
Hours of X-ray delivery to users

292
Ph.D. students among users

1191
Individual users (on site and remote)

637
Users on site

Guest house



1605 nights
Ukrainian residents (25 adults, 5 kids)

3263 nights
Users

7.1 nights
Average length of stay

6144 nights
Total

Food and drinks

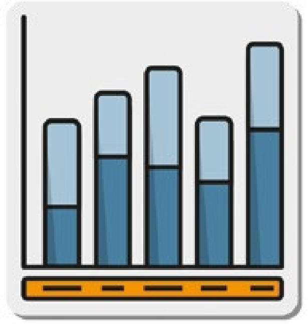
34 004
Sold meals

5781 kg
Used fruits and vegetables

3364
Sold Franzbrötchen

4514 l = 23 756 cups
Consumed coffee

1.25 t = 1250 kg = 6000 pieces
Free apples and pears for staff



Data

27.6
PB raw data collected

1.77 million hours
Cumulative time used for data analysis on the computing cluster

Zoom video conferencing

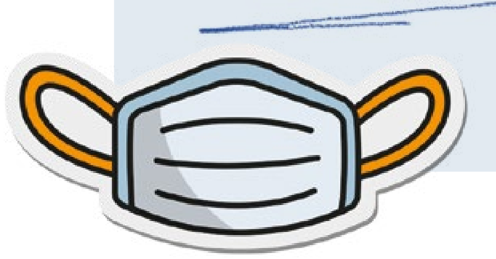
528
Active Zoom users

25
Webinars

131 064
Meeting hours

62 907
Meetings

Protective COVID-19 measures



7200
Surgery masks ordered

22 004
FFP2 masks ordered

26 000
Antigen test kits used

OPERATIONS

Inside Interaction Chamber 1 at the HED instrument

OPERATIONS

In many ways, 2022 was the first year of full operation of the European XFEL, following the buildup phase of the facility, on the one hand, and the constraints imposed by the COVID-19 pandemic, on the other. The year was marked by a huge increase in both the time delivered to the user programme and the number of user experiments. Operation was very reliable overall, with the exception of a few interruptions in early summer.

The performance of the European XFEL accelerator complex has matured greatly over the years. In 2022, the accelerator delivered electrons at energies ranging from 8.0 to 16.5 GeV, serving the ever-varying operational needs of the facility. The accelerator complex—consisting of an injector, a 17.5 GeV superconducting linear accelerator, an electron beam distribution system, and a beam transport system through the three SASE undulators to the beam dumps—was operated for nearly 7300 h (Figures 1 and 2).

Of these 7300 h, around 4400 were allocated to X-ray delivery, enabling operation of the scientific instruments with X-ray beam. Another 2250 h were used to set up and tune the accelerator and the undulators to meet standard operation parameters and specific experiment requirements. Alongside the two annual maintenance periods, this relatively large number of hours arises from the complexity of the accelerator and its subsystems as well as from the many different modes in which the accelerator and the undulators are operated to serve the needs of the users. A little less than 9% of annual operation hours was dedicated to further facility development, which covered activities in many different areas of the accelerator, FEL, and photon systems (Figure 3).

The overall availability of the facility was excellent—92.8% averaged over all the undulators—but slightly below the target of 95%. The main reason was failures of bearings in the cold compressors of the cryogenic plant, leading to several interruptions of operations in May, June, and July. Tests of new magnetic bearings to resolve this long-standing issue began at the end of 2022. Interruptions were also caused by trips of the radio frequency (RF) electron source (gun) in the injector related to a lifetime issue of the RF window. The window was exchanged in the summer maintenance period, thus eliminating the problem.

Several improvements, extensions, and European XFEL "firsts" were realized in 2022. For example, a new record for the electron beam power of 120 kW was achieved. The range of X-ray photon energies (or wavelengths) delivered to the scientific instruments was also extended to a factor of about 100, reaching from 260 eV (around 4.7 nm) to 30 keV (around 0.4 nm). X-rays with the lowest energies of 260 eV were generated by operating the accelerator at 8 GeV electron beam energy using the SASE3 undulator, while the highest X-ray energies of 30 keV were produced when operating at 16.5 GeV electron beam energy using SASE2.

During X-ray delivery for user experiments, the accelerator and the undulators were increasingly run in non-standard operation modes, which were introduced and tested before being made available for user operation. While these special modes generally require more time for setup and retuning, and performance is less predictable, good progress has been made using them. For example, hard X-ray self-seeding at SASE2 and the generation of two different wavelengths (two-colour mode) at SASE2 and SASE3 are special modes that can now nearly be considered standard.

The user requirement for extremely short X-ray pulse durations—of a few femtoseconds or even less than one femtosecond—has driven many development activities and will continue to be a research topic in the coming years. In 2022, the accelerator and the SASE3 undulator were run in a special mode providing ultrashort pulse durations. Using this mode, X-ray pulses with durations below 1 fs were measured in an experiment at the SQS instrument (see Facility Development on page 58 and refer to the SQS highlight on page 15).

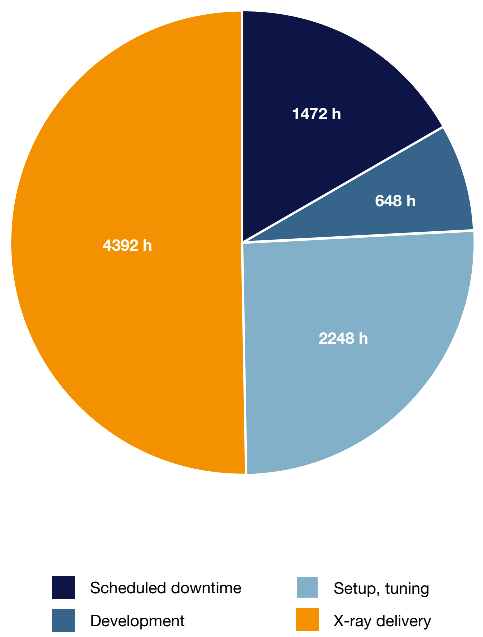


Figure 1:
Distribution of yearly operation hours of the European XFEL accelerator in four categories

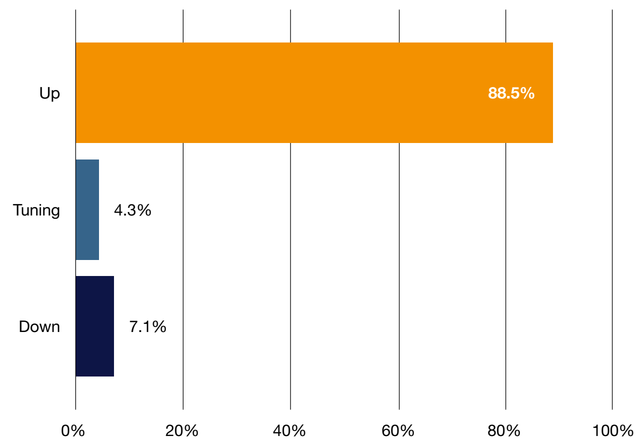


Figure 2:
Availability of the accelerator during X-ray delivery in percent

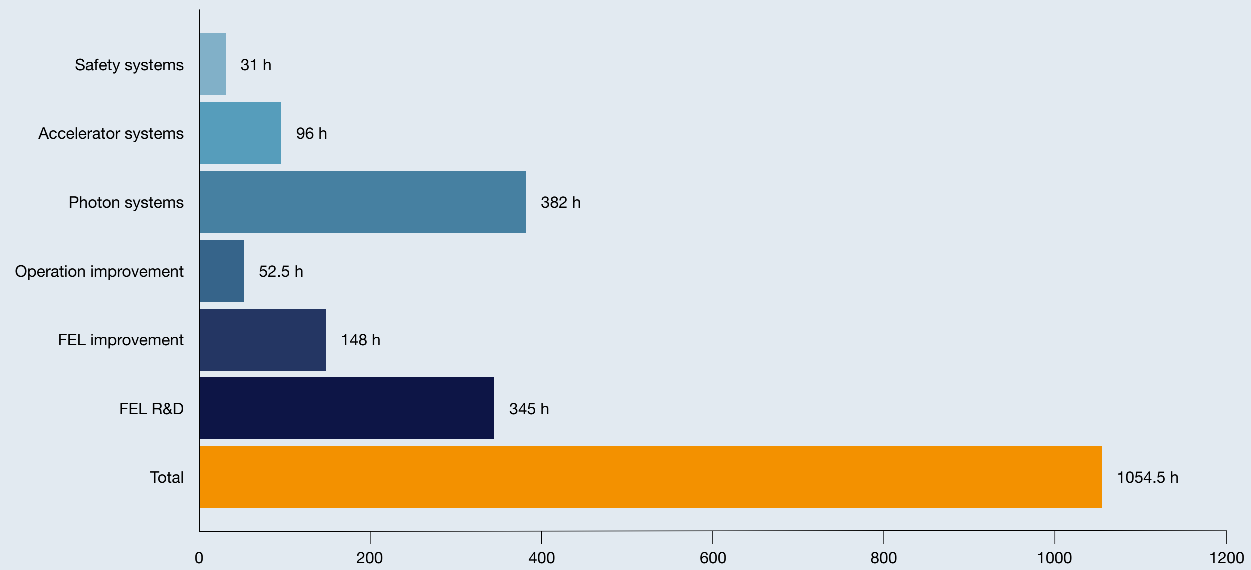


Figure 3:
Distribution of development time in hours. The sum of development hours scheduled for various facility development activities exceeds the hours for development indicated in Figure 1, reflecting the parallel use of the facility for multiple activities.

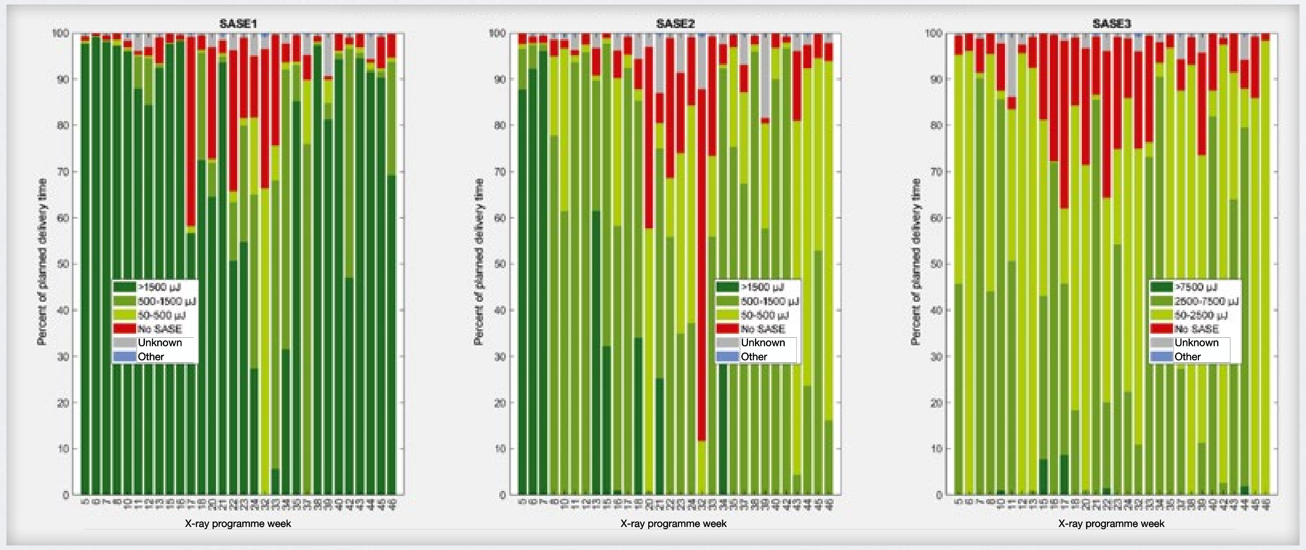
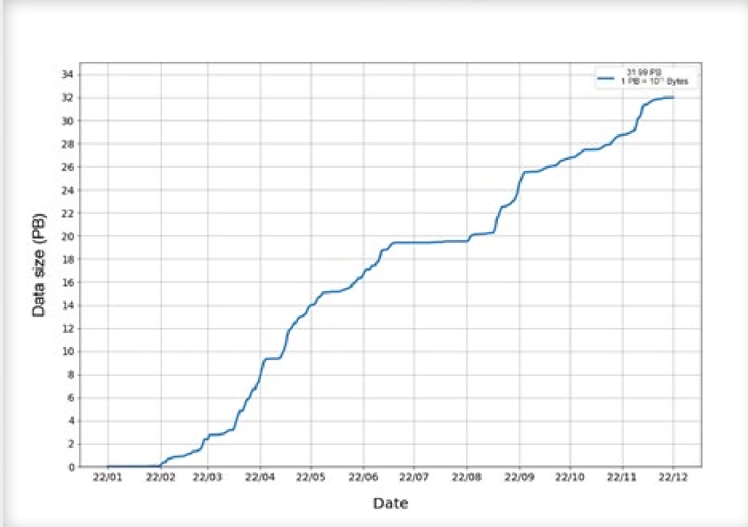


Figure 4:
Statistics of pulse energies provided by the three undulators SASE1, SASE2, and SASE3 during X-ray delivery in 2022



Instrument	Raw data (PB)
SPB/SFX	15
FXE	1.6
MID	11
HED	1.0
SCS	1.8
SQS	1.4

Figure 5:
Increase of raw data stored as a result of European XFEL operation in 2022 and distribution over the six scientific instruments

It remains challenging to offer standard and special mode operation in parallel at the different undulators, while maintaining stable operation to ensure a high stability of beam delivery. The very successful introduction of "beam regions" within the 600 µs long RF pulse in summer 2022 allowed the operators to achieve a much higher flexibility in setting the RF parameters required for the different operation modes, thereby providing a major step towards more independent operation of the undulators. Furthermore, additional kicker systems in the injector and improved operation of the fast longitudinal feedback system stabilized the time arrival properties of the long bunch trains.

On the photon systems side, operations were similarly successful. A clear highlight was the ability to increase the number of performed user experiments at the three beamlines to just under 100. The successful execution of experiments at the scientific instruments depends on an adequate delivery of the X-ray beam. In the past, and continuing into 2022, issues with beam delivery had occasionally rendered the X-ray delivery time partially or even entirely unusable for the instruments. In 2022, steps were taken to quantify the properties of the delivered X-rays, with the aim both to better define the expectations by users and scientific instrument staff and to identify deviations from the expected beam delivery.

So far, the only available parameter used to quantify beam delivery has been the X-ray pulse energy, measured by the X-ray gas monitors. This parameter has only limited meaning, however, because, when operated in special modes, the undulators typically generate less pulse energy than maximally possible in favour of other X-ray beam properties requested by the scientific programme. Other parameters—spatial beam position, X-ray photon energy and bandwidth, and X-ray pulse arrival time at the instruments—as well as the fluctuation of these parameters with time were therefore identified as necessary for quantifying the beam delivery more consistently.

An activity called Stable Operation Mission was started in 2022, with the task of establishing continued monitoring of the beam delivery parameters and addressing events in which strong deviation from the mean values were observed. Implementation of these measures is still ongoing, with only the pulse energy values being systematically retrieved in 2022 (Figure 4). To support the project, an experiment hall control room was set up, enabling monitoring of the X-ray beam delivery and improvement of the beam transport systems in parallel with operation. This room is also the base for the experiment hall crew, which supports the operation of the hall and the scientific instruments located within it.

An important part of operating the European XFEL is to manage the data acquired at the scientific instruments and in other parts of the facility. The infrastructure and processes dealing with this task for the photon systems have become highly mature in recent years. In 2022, approximately 30 PB of raw data were accumulated (Figure 5). By far the biggest sources of these data were the megapixel detectors installed at several of the scientific instruments, leading to a non-uniform distribution of data volumes.

In 2022, 95 individual experiments were allocated across the six scientific instruments (Figure 6). This number included seven protein crystal screening experiments, performed at SPB/SFX. All of these experiments were scheduled for beamtime after successful evaluation by the corresponding Project Review Panels in fall 2021 and spring 2022. A few experiments that could not be performed before, due to COVID-19 regulations or technical difficulties, have been allocated in 2022..

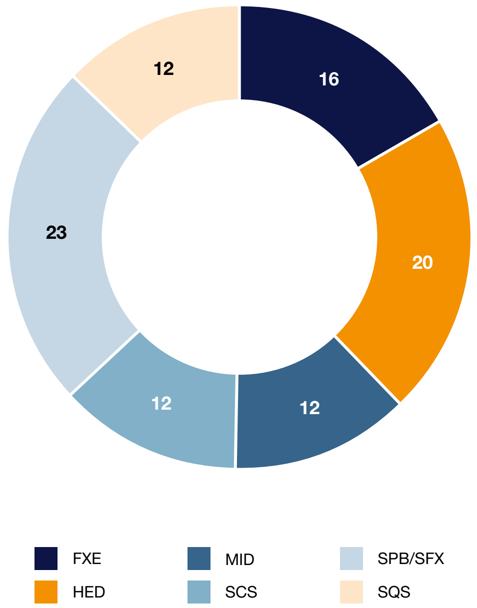


Figure 6:
Number of user experiments at the six scientific instruments in 2022

A total of 8080 h of X-ray delivery beamtime was allocated to these 95 experiments, close to an average of 85 h per experiment. In some cases, this time included the preparation of the instrument for the corresponding user experiment. A total of 1191 individual users contributed to a total of 1944 user visits, including both onsite presence and remote access to the facility (Figures 7 to 10). A large fraction of user visits still occurred through remote access, although 637 researchers came for 849 in-person visits. The average number of users participating in person per experiment was 9, a fairly high number considering the still noticeable impact of COVID-related travel and access restrictions.

European XFEL issued two new calls for proposals for experiments to be carried out at the facility in 2023. These calls included the possibility to propose regular experiments or to make long-term proposals. A topical call was also launched, focused on experiments on molecular water research. This call was aimed at a wider community of scientific groups addressing molecular water research, in particular scientists who were not experts or frequent users of FEL facilities. It consisted of a two-stage proposal process with an initial letter of intent, a preliminary review, and a subsequent full proposal as part of the first call of 2022.

The call for long-term proposals was aimed at establishing new X-ray techniques or instrumentation that will benefit the science programme in the longer term. In addition, the possibility for protein crystal screening proposals at SPB/SFX was offered in the first and second calls of 2022. The overall outcome of the two calls for proposals was very successful, with the call for experiments to be performed in the first semester of 2023 hitting an over-subscription factor of close to 4. Very high-ranked molecular water science and long-term proposals were allocated at all of the scientific instruments.

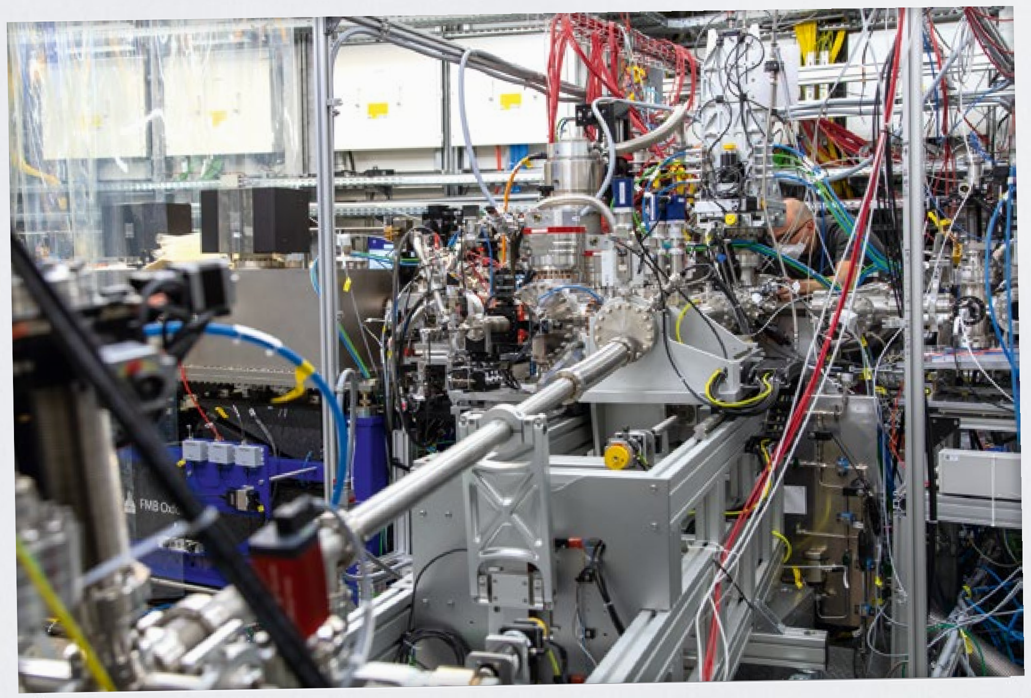


Figure 7:
Researchers from European XFEL and Uppsala University preparing the new 1D imaging XUV spectrometer at the SQS instrument

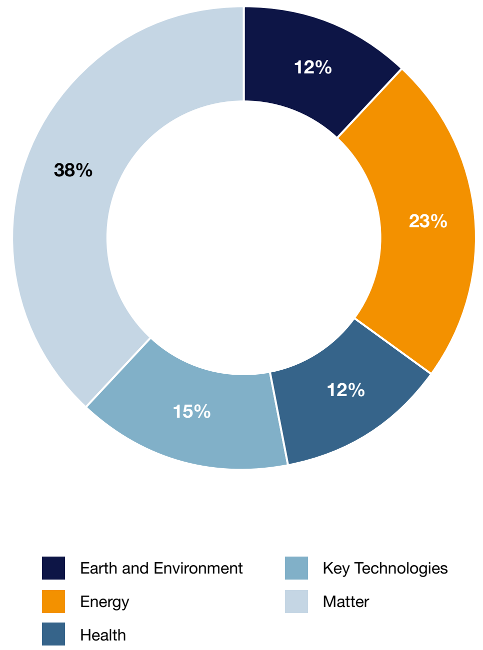


Figure 8:
Distribution of users according to societal challenges as identified by European XFEL

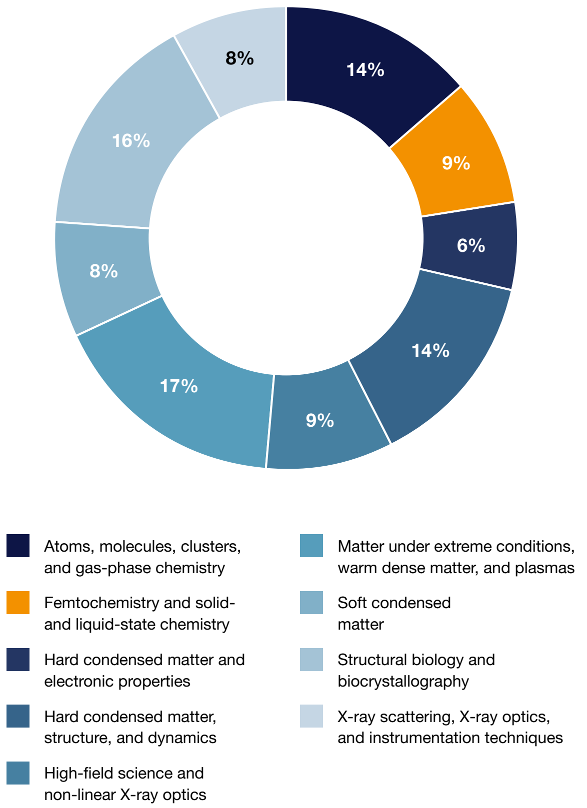


Figure 9:
Distribution of users according to major scientific areas

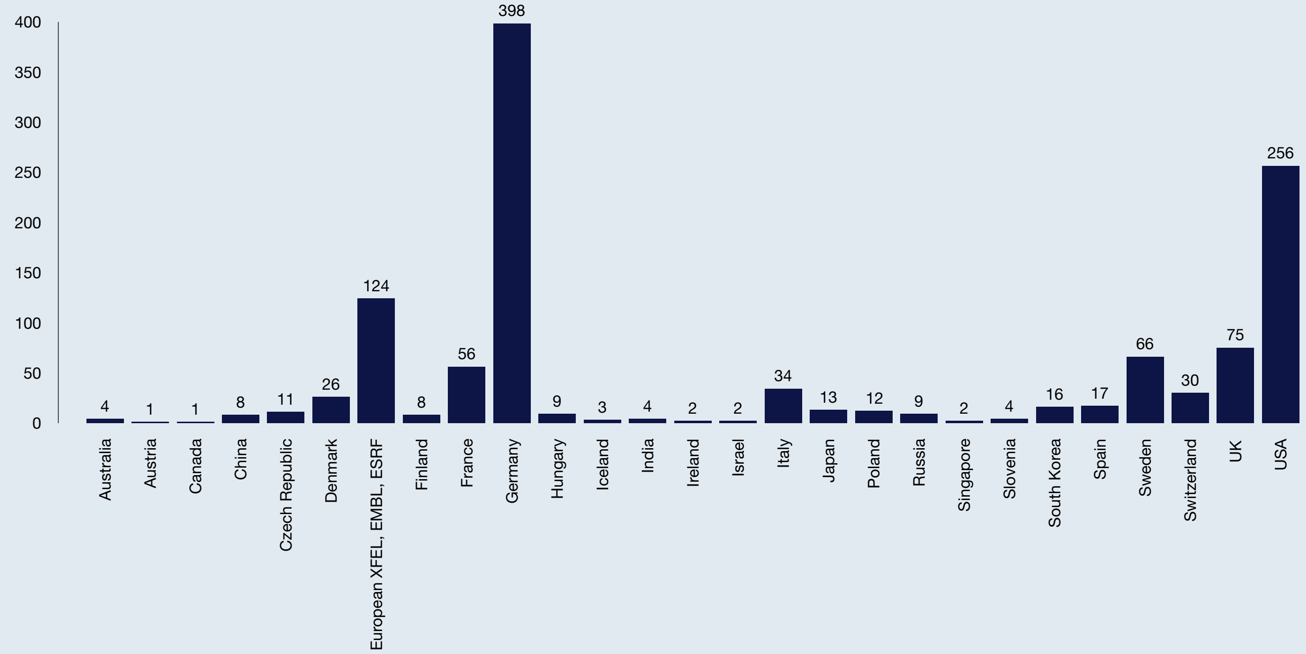


Figure 10:
Country of affiliation of the 1191 individual users who participated in experiments in 2022. Users of the international facilities European XFEL, EMBL, and ESRF are listed separately.

FACILITY UPDATE

Celebrating the topping-out ceremony for a new office complex on the Schenefeld campus

CAMPUS DEVELOPMENT

In 2022, there were two major activity areas of campus development: the further completion of buildings and infrastructure and the review and improvement of energy consumption.

Improving the experiment hall

Several actions were taken to improve the installations in the experiment hall, XHEXP. The biggest was to begin construction of a new compressed-air distribution system, consisting of a new compressor room in the adjacent ventilation and air conditioning building, XHVAC, and a new ring line. This line supplies XHEXP, the scientific instruments, and the laser hutches with compressed air at a pressure of 15 bar. A new room to host the large capacitor bank for the Helmholtz International Beamline for Extreme Fields (HiBEF) pulsed-magnet system at the HED instrument was built, and the installation of the pulser was started. A new control room for the XHEXP hall crew and for beam transport system operation was set up in XHEXP as well.

On the laboratory floor of the headquearters building, XHQ, the central argon supply was rebuilt, a secondary treatment plant for high-purity water was installed, and part of the XBI biology laboratories were remodelled. In addition, for all buildings on campus, a new building management tool was installed, commissioned, and taken into operation. This software receives signals from and interacts with most technical infrastructure on campus. It thus allows technical staff to significantly increase the operational stability, while enabling an optimal performance of the various technical infrastructure systems.

Expanding the campus

Construction and infrastructure work focused on the western part of the Schenefeld campus. Here, the construction of the second office building, XHO, progressed quickly throughout the year. The topping-out ceremony for the building was celebrated on 25 March and, towards the end of the year, acceptance tests were started on most of the building. Through careful planning and early procurement of critical construction materials, it was possible to complete XHO almost on schedule and within the planned costs. Commissioning of the electrical infrastructure, however, needed to be delayed until spring 2023 due to extended delivery times for the sub-distribution boards for the power supply. This will amount to a delay of up to two months compared to the initial timeline.

Figure 1 :
Top: HiBEF pulser at HED. Bottom: XHEXP control room

Figure 2:
Construction begins on the visitor and conference centre.

Figure 3:
European XFEL Managing Director Robert Feidenhans'l and spectrometry scientist Naresh Kujala began to establish a new garden next to the company restaurant.

For XHO and the visitor and conference centre, XHV, the technical infrastructure in the western part of the campus area had to be expanded. Heating and cooling lines for the future buildings were installed, and the site's freshwater and drainage systems were extended. The electricity and equivalent network supply were also decisively improved by the installation of a new transformer and further sub-distribution boards for this area. The earthwork and the laying of underground lines for XHV began toward the end of 2022.

An outdoor activity to improve the campus was to create a small garden for flowers and vegetables near the company restaurant, BeamStop. This activity is entirely driven and supported by European XFEL staff members.

Improving energy consumption

Reviewing and improving energy consumption was also an important area of activity in 2022. The Schenefeld campus, of all European XFEL installations, accounts for around 15% of the facility's overall energy consumption. Part of this fraction is needed for the supply of tunnel operation and of the systems in them. Another energy resource used on the Schenefeld campus is heat, provided by the district heating system.

Over the past years, optimization of the heating systems created a better heat balance. Through optimization, stabilization, and energy-saving measures, the heat demand was reduced to almost half its original value between 2019 and 2022, despite two additional buildings in need of supply. The increased German energy-saving requirements were quickly implemented thanks to the new building management tool.

In order to increase overall energy sustainability and respond to the increase in energy market prices, the consumption of the overall facility was reviewed during the year. For the Schenefeld campus, a 10% reduction in electrical energy consumption was defined as a target, and a task force was established in November to find and evaluate potential savings in machine parameters or in secondary technical infrastructure. However, since the facility has been in the buildup phase, while at the same time seeing operation restrictions due to the COVID-19 pandemic, it is not simple to determine a reference value. In many ways, 2022 was the first year of full operation and, at the same time, the first year in which energy conservation measures were applied. An analysis of the years 2021 and 2022 shows an annual electricity consumption of approximately 15.5 GWh for the Schenefeld campus.

FACILITY DEVELOPMENT

While operation of the facility is the main activity of European XFEL, development activities are also undertaken to improve the performance of existing systems and to enable the use of new working points and instrumentation. These development activities take place across all areas of the facility, with specific improvements made in 2022 to the accelerator, undulators, beam transport systems, and scientific instruments.

Accelerator, undulators, and X-ray beam transport systems

Some of the measures to improve the accelerator, undulators, and X-ray beam transport systems immediately yielded new record performance, for example in terms of FEL photon energies, average intensities, or X-ray pulse duration. Other activities were aimed at long-term goals and served to prepare for new installations or new operation modes.

A particular activity that combined the efforts of accelerator, FEL, and X-ray system experts was the programme to provide extremely short X-ray pulses, with durations from a few femtoseconds down to the attosecond range. In 2022, specific hardware was not yet installed to support this mode of operation. However, several hardware-free methods for generating soft and hard X-ray pulses with femtosecond to sub-femtosecond duration were investigated. The next step will be to install
dedicated hardware that allows the best possible control of the bunch lasing window below the coherence time limit. These efforts are bundled in the Attosecond Pulses with Enhanced SASE and Chirp/Taper (ASPECT) project.

In 2022, two methods for X-ray pulse duration control were implemented, combined, and customized for use at the different undulators. The first method employs two stages: the variation of the charge of each electron bunch produced by the electron source (gun) in combination with optimized compression of the bunch (Figure 1). In the first stage, an acousto-optical modulator (AOM) in the gun laser makes it possible to generate bunches with variable charge along the bunch train. Since the AOM operates at 4.5 MHz, the system is able to customize the bunch charge for each electron bunch dedicated to lase in any of the three undulators. In the second stage, the radio frequency (RF) system is used to modulate the energy “chirp”, or spread, and thus the compression of the electron bunches in the train. This stage is limited in terms of interoperability of the beamlines due to transition times of tens of microseconds, but work to reduce this limitation is ongoing. Combining these two stages, the first method is simple, allows for individual X-ray pulse duration control for each undulator, and was implemented for user operation. No interference with the operation of the other undulators was experienced, and X-ray pulses with single-peak spectra were observed, corresponding to ultrashort pulse durations (Figure 2).

The second method to produce ultrashort X-ray pulses employs dispersive settings in the SASE3 FEL undulator. The low photon energies at SASE3 allow for lasing with relaxed electron beam characteristics compared to SASE1 and SASE2, and, at around 1 keV, lasing can be supported by electron beams with higher peak currents than in the nominal case. These peak currents are obtained by more aggressive than usual compression settings, resulting in complex longitudinal phase space properties. When dispersion is added in the undulator, a situation can be created in which only a thin slice of the electron bunch travels on a straight trajectory through the FEL, thus contributing to lasing. As a result, ultrashort X-ray pulses with relatively high pulse energy are produced (Figure 3). A dedicated measurement campaign based on angular streaking has confirmed pulse durations of approximately 700 as.

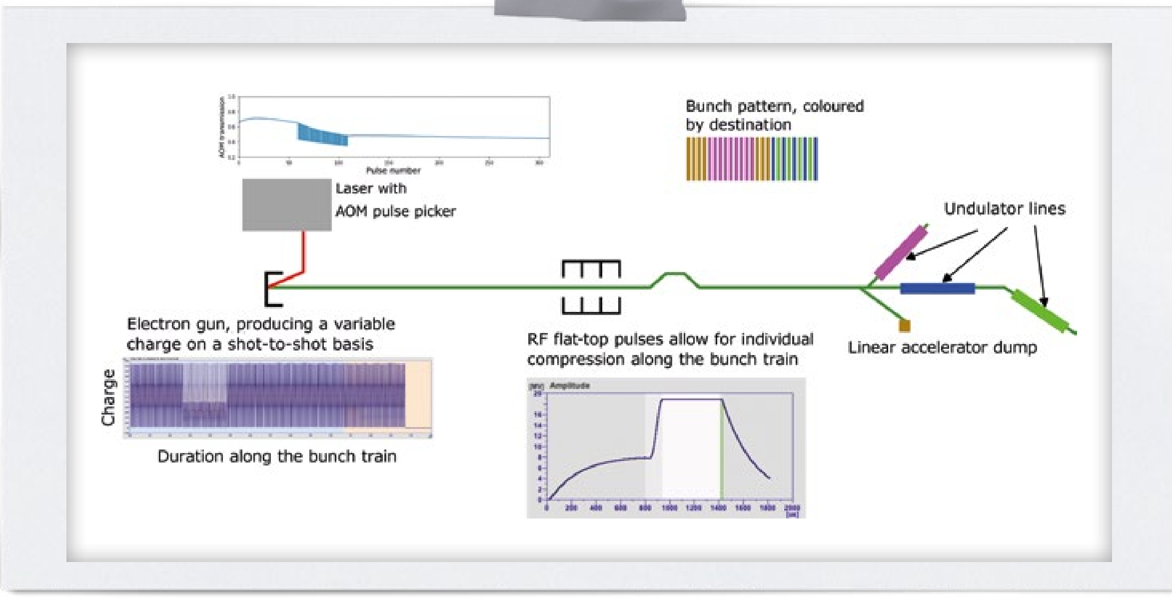


Figure 1:
Schematic layout of the European XFEL with its electron bunch trains feeding the three FEL undulator lines. The laser AOM absorber located close to the electron gun makes it possible to arbitrarily shape the charge profile of the electron bunches. The modulated RF flat-top pulse allows for individual bunch compression along the train.

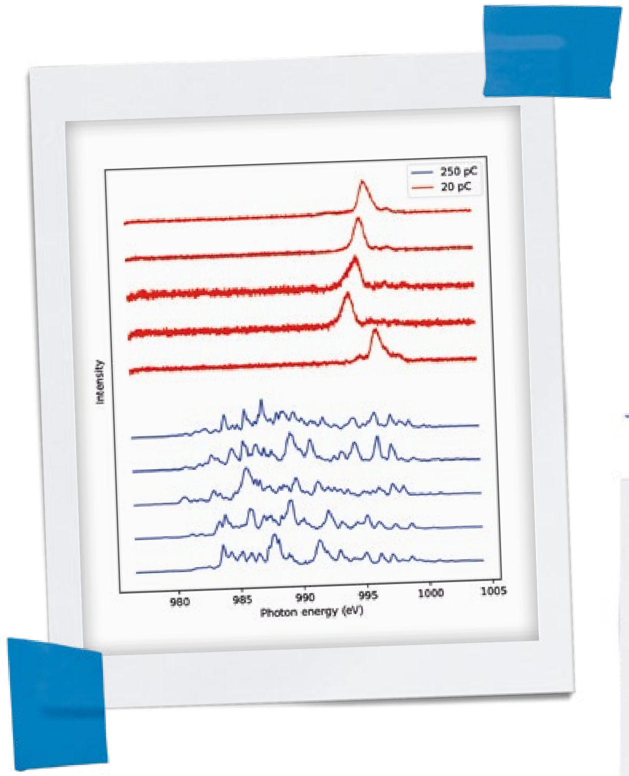


Figure 2:
Selected X-ray spectra for nominal (250 pC, blue) and low-charge (20 pC, red) electron bunches with optimized electron bunch compression settings

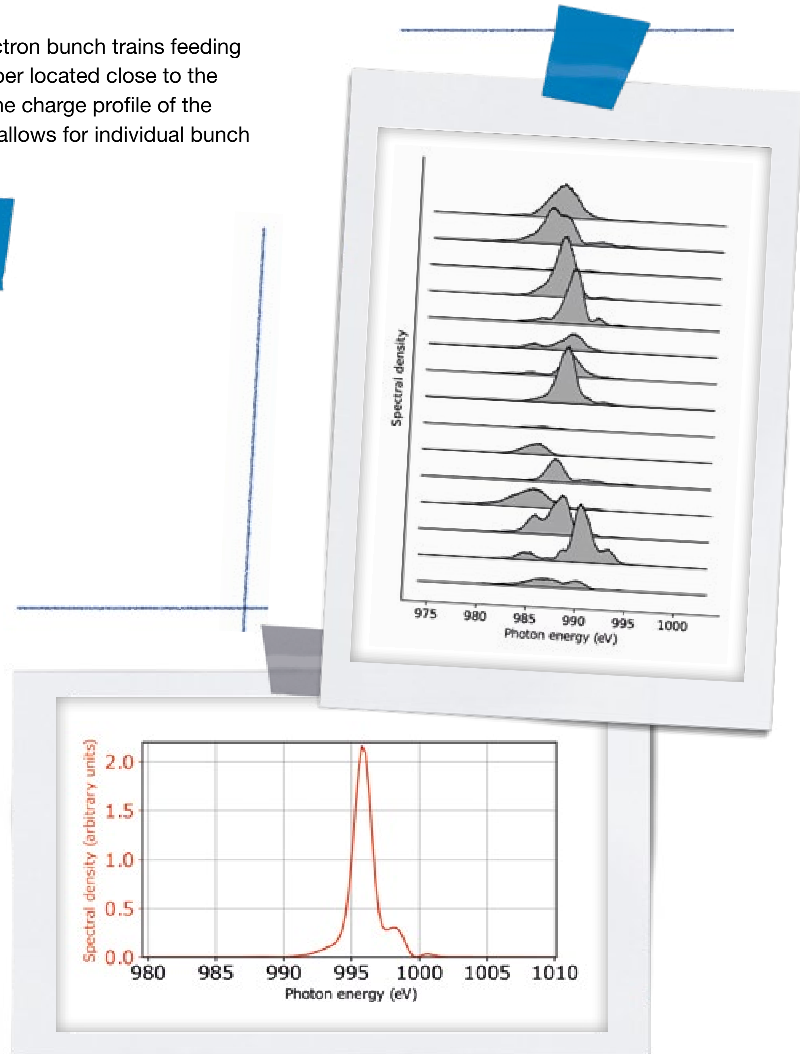


Figure 3:
Top: Ten consecutive measurements of nearly single-spike X-ray spectra at an averaged pulse energy of 600 µJ (June 2022).
Bottom: Simulation of the spectrum of an ultrashort X-ray pulse produced by over-compression and dispersive settings.

Towards the end of 2022 and during the winter maintenance period, several new devices and systems were installed to prepare for new operational and performance features. One of them is a “dechirper”—a device based on a corrugated structure that delivers a time-dependent transverse kick to the electron bunches—which was installed before the SASE1 FEL undulator. The dechirper will support the generation of ultrashort pulses and provide additional diagnostics. Another major activity was the modification of the electron beamline in front of SASE1 over a length of 50 m to prepare for installations within the ASPECT project. First diagnostic devices for the X-ray free-electron laser oscillator (XFELO) demo experiment at SASE1 were also installed.

Test operation of the first active magnetic bearing in one of the cold helium compressors of the cryogenic plant started at the beginning of the winter maintenance period. The commissioning and initial operation of the new bearings were successful, giving hope that the long-standing problem with the bearings used to date, which led to several interruptions of operations in May, June, and July 2022, can be resolved. However, long-term tests must continue in order to demonstrate the anticipated many 1000 hours lifetime of the new bearings, and the full refitting of the cold compressors with magnetic bearings will require a few years.

Preparations for the further development and extension of the European XFEL facility are also ongoing. Construction of the electron gun conditioning facility FALCO should be completed in 2023, and R&D work for the systems required to upgrade the accelerator for operation in continuous-wave mode is in full swing.
In terms of the development of the FEL sources, four APPLE-X undulators forming a “helical afterburner” for the generation of X-rays with freely adjustable polarization were installed behind the SASE3 undulator during the winter maintenance period 2021–2022, and their initial commissioning began in early 2022. In May, circular polarized radiation was observed at a photon energy of around 1 keV. However, soon afterwards, motion control of the undulator segments became impossible due to radiation damage of encoders and motors installed on the devices. As the cause of radiation was not clear and repair was not possible on site due to the very tight installation space, all the devices were dismounted in the summer maintenance period. Later, spontaneous synchrotron radiation generated in the upstream SASE3 undulator was identified as the root cause of the radiation damage. In the second half of 2022, the APPLE-X undulators were remeasured to confirm that the magnetic structures had not been damaged by the radiation, and measurements were performed to quantitatively better understand the background radiation. In the winter maintenance period 2022–2023, a narrow chamber of the same dimensions was installed behind SASE3 to demonstrate that the radiation background is controllable.
Re-installation of the APPLE-X undulators is planned for the winter maintenance period 2023.

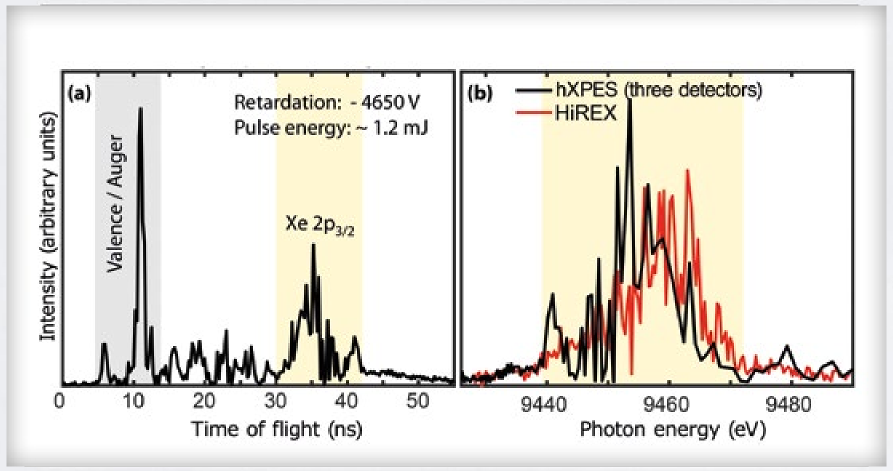


Figure 4:
SASE1 hXPES online measurement of X-ray pulse spectra, taken in 20-pulse mode with an intra-train repetition rate of 0.25 MHz and an average pulse energy of 1.2 mJ. Left: Single-shot time-of-flight spectrum. Right: Photon energy spectrum. The spectrum in red was obtained simultaneously with the HiREX spectrometer.

In recent months, many groups have been working intensively on ways to reduce energy consumption. The RF system of the accelerator is now being operated in a more adapted and thus more economical way, and other infrastructure is also being optimized for more efficient usage. On average, it should be possible to save 5–10% of the roughly 12 MW of electrical power used when the European XFEL facility is operated at full energy.

To improve the online diagnostic capabilities for the hard X-ray beam transport systems, a hard X-ray photoelectron spectrometer (hXPES) was installed and commissioned in the SASE1 beamline. The device provides single-shot non-invasive spectral diagnostics in the range of 4–20 keV with 10 eV resolution and thus complements the crystal-based, partially invasive, high-resolution hard X-ray single-shot (HiREX) spectrometer. The hXPES has several detectors that record time-of-flight spectra of photoelectrons emitted by residual gas hit by the X-ray pulse. Signals from several detectors can be combined to increase the single-pulse signal-to-noise performance. Time-of-flight spectra are converted by software to photon energy spectra according to a calibration function (Figure 4).

Another R&D project focused on the development of diamond sensors as nearly non-invasive position and intensity detectors for hard X-rays, enabling 4.5 MHz operation. Here, a diamond sensor—consisting of a 40 µm electronic-grade single-crystal CVD diamond with graphitized surfaces and duo lateral electrode geometry—was tested in the SASE2 beamline at a photon energy of 30 keV. The preliminary results show that the diamond sensor delivers pulse-resolved X-ray beam position and intensity measurements at 2.25 MHz, and the results are in good agreement with measurements by the adjacent FEL imager and X-ray gas monitor (Figure 5).

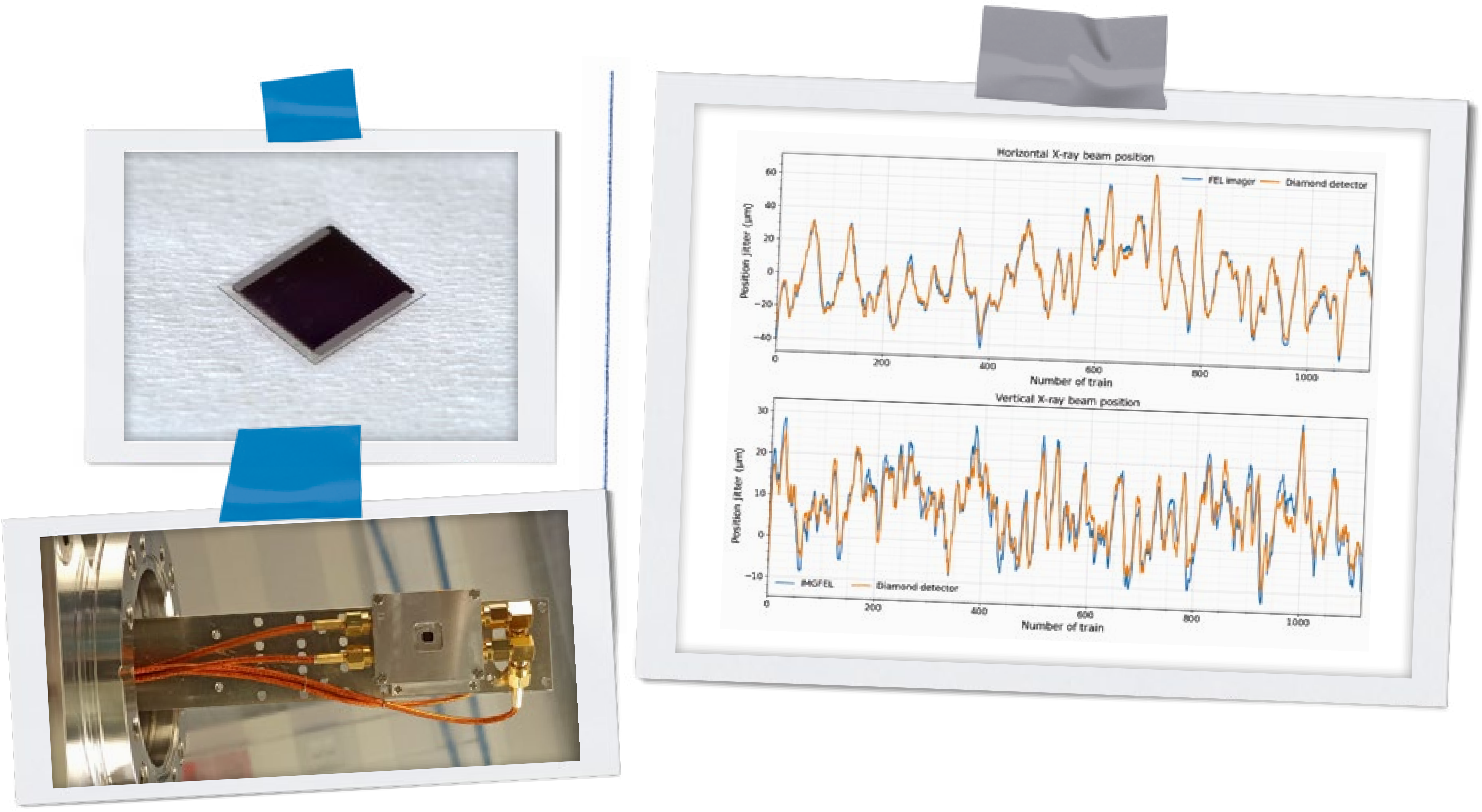


Figure 5:
Left: Diamond detector setup in the K-monochromator chamber of SASE2.
Right: Measurements of the horizontal (top) and vertical (bottom) X-ray beam positions made with the diamond detector (orange) compared to those provided by an adjacent FEL imager (blue).
For smoothing, the signal was averaged over two X-ray pulses, and a Savitsky–Golay filter was applied.

Another R&D project addressed the problem that the installed hard X-ray monochromators show a significant decrease of the transmitted intensity with increasing number of pulses, which is due to the high repetition rate and pulse energy of the X-ray beams. As a material, diamond combines the best thermal conductivity with low thermal expansion. When crystals of sufficient quality and size recently became available, a project to build a high-heat-load monochromator was initiated. For this, an all-diamond channel-cut monochromator (DCCM) was designed (Figure 6), and its performance was simulated through finite-element calculations. The DDCM was procured externally and characterized using collimated high-energy X-rays at synchrotron sources. In 2022, the prototype DCCM was tested at the MID and FXE beamlines under full X-ray beam load at room temperature, demonstrating the ability to maintain a high throughput over an entire X-ray pulse train and, subsequently, for multiple consecutive trains. This promising result confirms the high heat dissipation capability of diamond, which cannot be achieved with silicon, even under cryocooling conditions. The ultimate efficiency of the DCCM at cryogenic temperatures will be tested in 2023.

Scientific instruments

At the SQS instrument, a new spectrometer for analysing soft X-ray and extreme ultraviolet (XUV) radiation was put into operation (Figure 7). The 3.5 m long device was a Swedish in-kind contribution, built and implemented within a collaboration with Uppsala University. Anticipated since the start of the SQS instrument, the new XUV spectrometer will complement the already existing instrumentation at SQS, which is mainly dedicated to the analysis of electrons and ions. As a unique feature, a pair of cylindrical Wolter mirrors allows for one-dimensional (1D) imaging of an extended source. The XUV spectrometer can be installed in the F1' focus position of the Atomic-like Quantum Systems (AQS) chamber, replacing the magnetic-bottle spectrometer. A cylindrical grating mounted in the perpendicular plane provides energy dispersion so that the detector records an image with wavelength dispersion in one direction and spatial resolution in the other. The spectrometer covers the energy range of 140–1150 eV, with an energy resolution estimated to be about 70 meV at 250 eV and 100 meV at 540 eV. The device images a line source of up to 2 mm length with a resolution of 15 µm, allowing observation of the propagation effects of intense FEL radiation in dense gaseous media.

First commissioning experiments and a first user beamtime with the XUV spectrometer were successfully completed in November 2022, and the spectrometer's excellent performance was verified (Figure 8). The spectrometer will enable fresh avenues of research, especially regarding to the investigation of non-linear phenomena. The spectroscopy of XUV fluorescence photons emitted by a sample is a powerful tool for investigating photons that are not perturbed by the presence of charged particles, such as those commonly created in a sample's interaction volume.

Organizing development activities

In a facility like the European XFEL—with a strong user and experiment programme and related requests for support by other expert groups—it is necessary to define, structure, and approve any large development projects (DPs). In this way, adequate resources can be provided to support operation and new activities. At the beginning of 2022, 25 approved DPs were running. By the end of the year, 10 of these had been closed and 9 new DPs had started (Figure 9). The total budget of the new projects is approximately 1.7 million euro, with the XFELO project being by far the largest. Using the currently ongoing discussion of 11 new projects as an indicator, it is anticipated that the number of DPs will remain at its current level.

The Project Technical Coordinator (PTC) in the Data Department performs the important role of providing both oversight and an interface for the DPs. Each group in the Data Department has the latitude to define its own processes and procedures, and the PTC mediates the individual processes, acts as single interface to the Project Management Office and the managers of the DPs, and communicates and coordinates tasks within the department itself. The position was established at the beginning of 2021. Since then, the PTC has contributed to 34 DPs. While the coordination aspect is the most visible, the PTC also contributes expert advice to the implementation of new DPs as well as lessons learned from completed DPs, thus helping to improve the performance of the department.

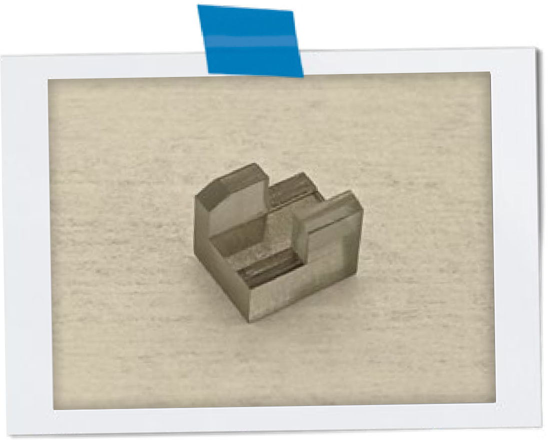


Figure 6:
Diamond channel-cut monochromator
(4 x 4 x 5 mm³) made of a single-crystal diamond

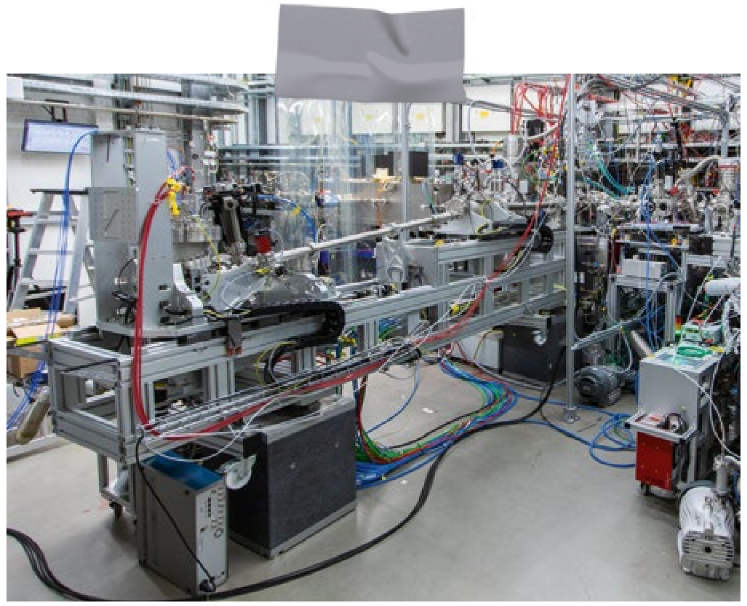


Figure 7:
New 1D-imaging XUV spectrometer installed at the SQS instrument

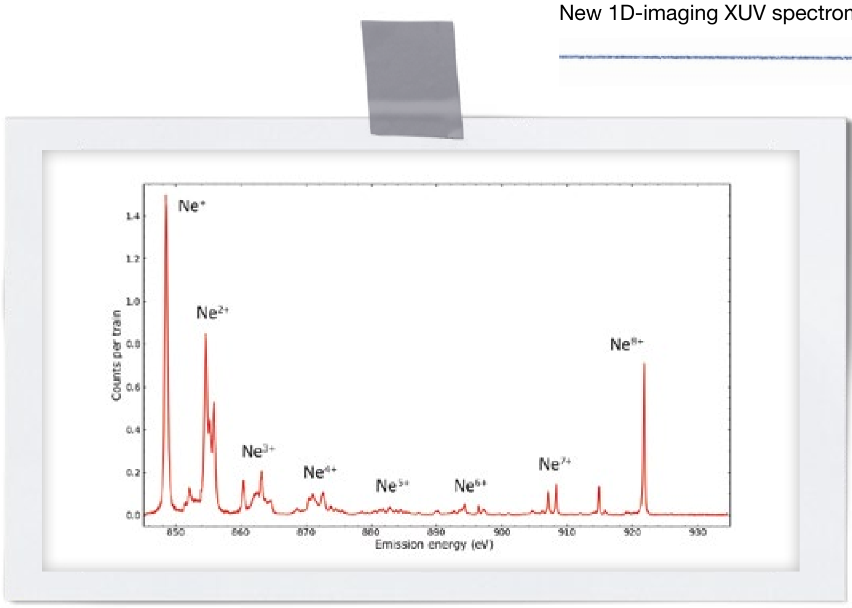


Figure 8:
Fluorescence spectra recorded with the XUV spectrometer upon excitation of neon gas with intense FEL radiation at 1.5 keV photon energy. The 2p → 1s emission lines from the different ionic states are indicated.

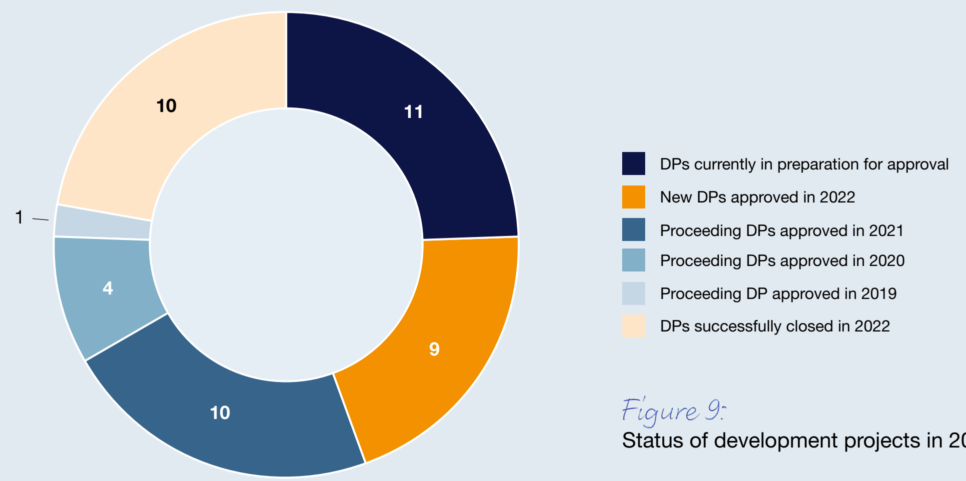


Figure 9:
Status of development projects in 2022

EUROPEAN XFEL STRATEGY

In 2020, European XFEL initiated an intense strategy development process, with the goal of defining the company's development targets for the coming decade. Five overarching Action Field teams have contributed to the strategy design process. Led by one European XFEL Director respectively, each team has worked on defining strategic goals for the coming decade, based on the facility development potential, scientific trends, megatrends, and user needs.

The strategy process aims to establish the basis for organizational transformation and vision for the next decade. Adding a challenge-driven approach to the discovery-driven science currently performed at European XFEL is expected to further increase the contributions to solving global societal challenges.

A *Strategy Design Report* is expected to be ready in 2023. An "Executive Summary" will be presented to and discussed with the European XFEL Council.

Development at European XFEL is also linked to development at its shareholder and partner, DESY. Consequently, synergies and areas where the strategic directions of the two facilities are complementary and where efforts can be combined successfully are regularly discussed at the directorate level.

Four societal challenges to which European XFEL could make significant contributions have been identified: Climate and Energy, Health, Environment and Sustainability, and Digitalization. The contributions will be based on strong science programmes across the instruments.

Strategy 2030 outlook

The mid-term European XFEL Strategy 2030 will address the timeframe until 2030 and restrict itself to the present accelerator layout.

European XFEL aims to make operation more efficient and increase capacity, expand its user base, achieve scientific excellence, and enhance company development. Furthermore, to maintain its technological leadership, European XFEL will continue research and development activities on new technologies and future upgrades.

A major upgrade of the facility, which will be necessary in the 2030s in order to enhance and maintain European XFEL's technological leadership, will be further investigated. The defining elements are an upgrade of the accelerator, and a second fan of photon tunnels with a beam distribution building and a second experiment hall. This would allow the company to build more instruments dedicated to specific applications and to serve the growing user community.

Figure 1:
Action Fields of the strategy process

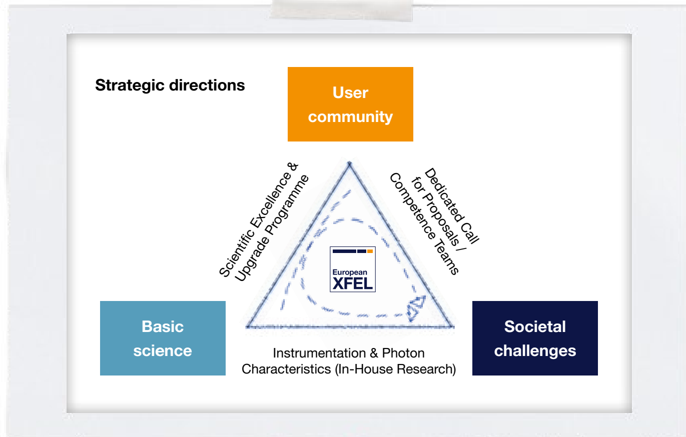


Figure 2:
Diagram illustrating the interaction between the basic science programme, the user community, and the societal challenges

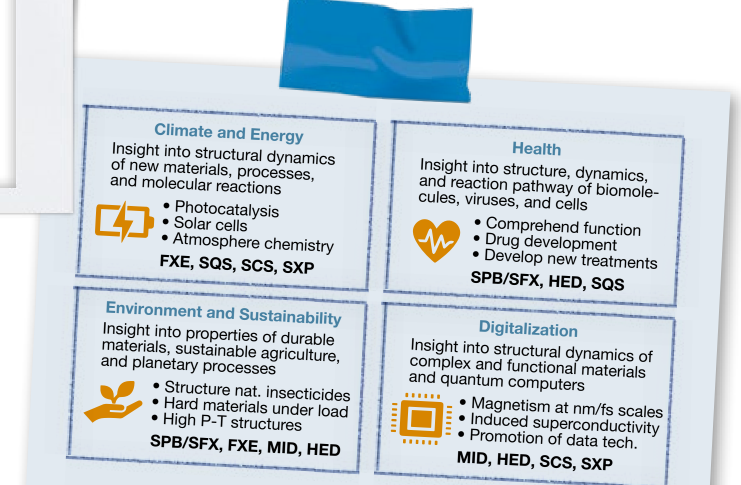
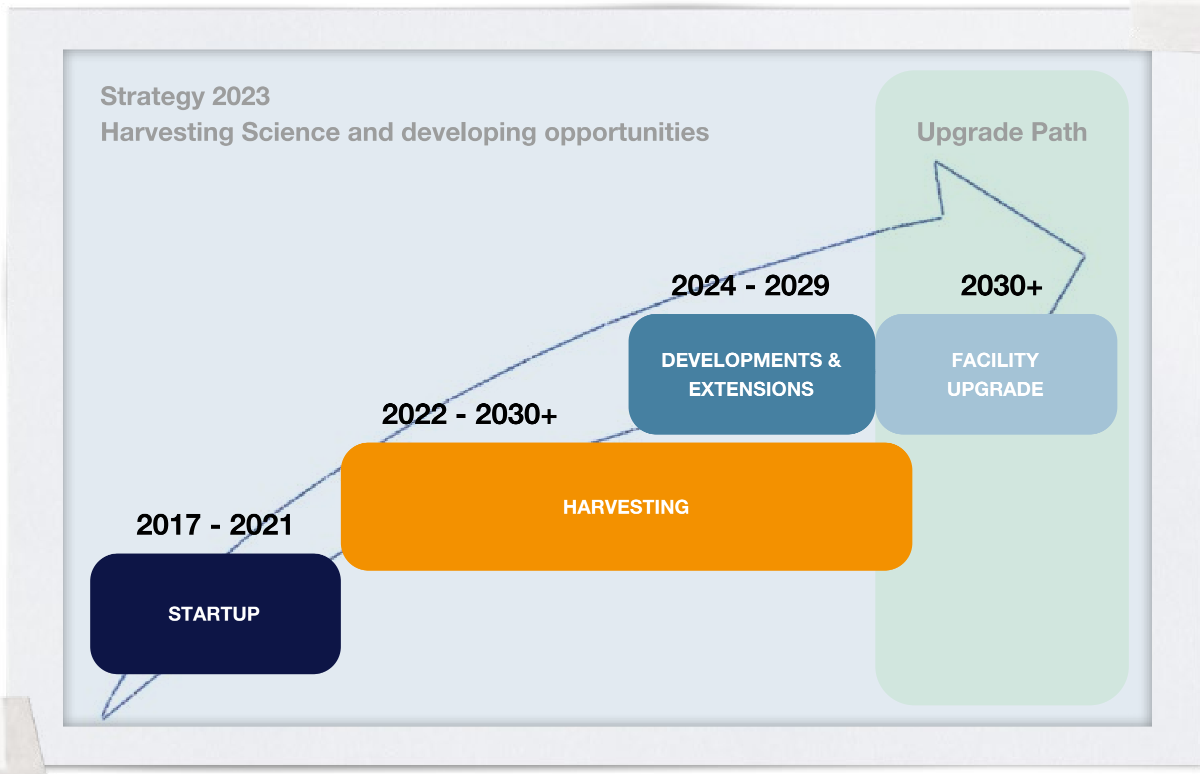


Figure 3:
Overview of the key societal challenges addressed by science experiments at the European XFEL, indicating which instruments contribute most prominently to these areas

Figure 4:
European XFEL Facility Roadmap



PERSONNEL DEVELOPMENT

European XFEL is committed to providing an environment in which people are able to fully develop their potential, regardless of their cultural background, physical abilities, or gender. Taking their individual strengths and competencies into consideration, staff members are to be trained in the skills and qualifications required to achieve optimal work performance. Through a variety of training sessions, workshops, and coaching sessions, every staff member is able to grow on a personal and professional level.

In 2022, European XFEL put special emphasis on training staff members in the further development of leadership skills.

Based on evaluations from the annual feedback talks, a soft skills catalogue was compiled. Training sessions supported staff members to reflect on themselves, exchange with others, and learn new skills. In addition, there was a great demand for team workshops. Topics that groups wanted to discuss included clarifying team goals, roles, and tasks, improving work procedures and processes, and dealing with conflict situations. At the same time, the team workshops were a great occasion to improve team spirit, build trust, and foster cooperation.

European XFEL rewards and recognizes staff members who use their broad range of experience and expertise not only to enhance their own performance but also to help their own group and the whole company achieve their objectives and missions.

Senior roles—seen as expert paths—were introduced as a new option for professional development at European XFEL. In addition, as part of the strategy process, a new leadership training format for group leaders was developed, and a pilot training was held in October 2022 with leaders from various areas of the facility.

As a next step, an extensive review of the Personnel Development learning and development provision is planned. The company will specifically invest in the development of conflict management and communication skills at all levels. It will also continue to build on a partnership approach between individuals and supervisors. The company's learning and development provision will recognize the diverse range of staff groups within the workforce and be tailored to meet their specific needs.

OUR VALUES

European XFEL's values—*collaboration, excellence, transparency,* and *trust*—are the core of our mission and strategy. Their purpose is to help express what we stand for and what is important to our facility. Defined in 2021 by a bottom-up process involving an extensive staff survey, the values aid European XFEL in building a supportive, inclusive, and highly motivating environment.

In the last 12 months, various activities were undertaken to highlight our values. Half-day workshops focusing on one value at a time were offered as part of the Personnel Development training catalogue. Internal awareness was also raised by the distribution of specially designed flower-seed packages, advent calendars, and water bottles.

A culture change agent network of 10 European XFEL staff members from a variety of professions and nationalities supports staff members in integrating the organization's values into their working lives.

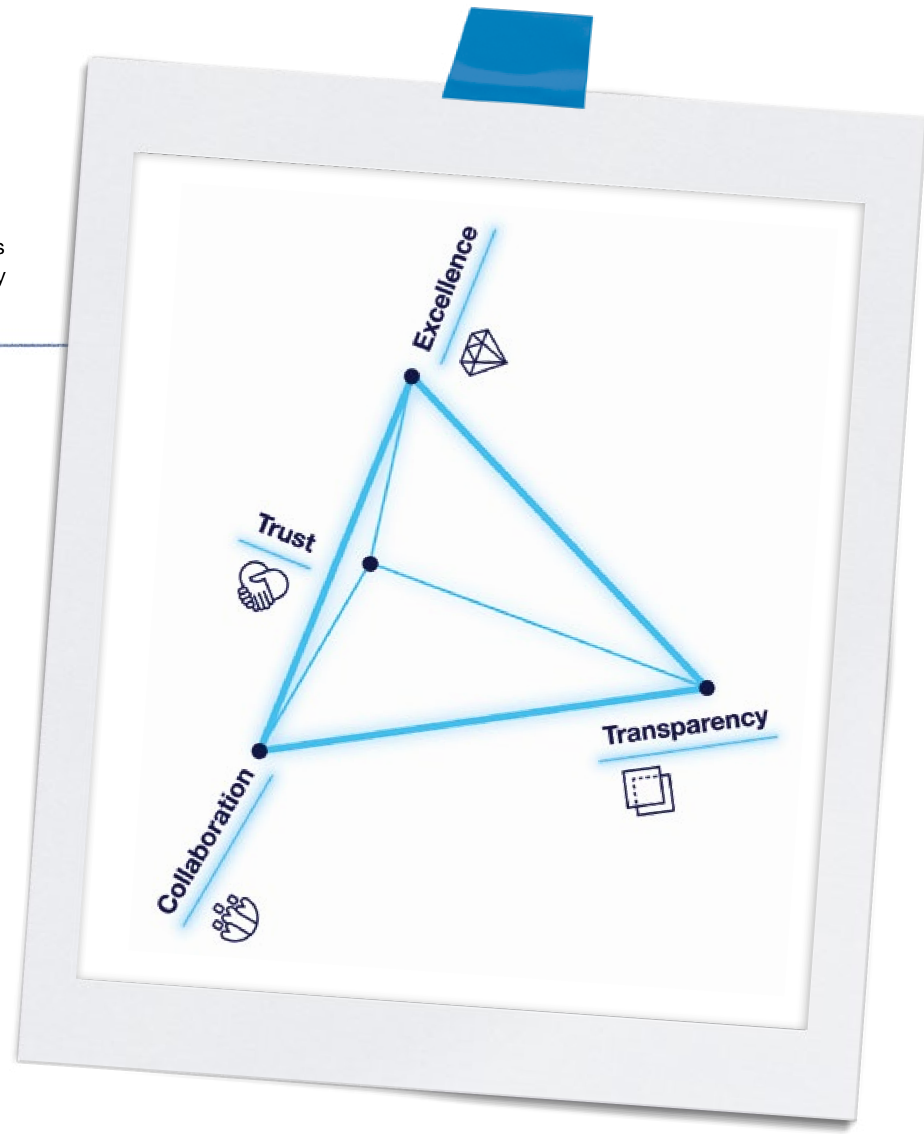


Figure 1: The European XFEL values—identified and defined by employees for employees

EUROPEAN XFEL Ph.D. PROGRAMME

The European XFEL Ph.D. programme is designed to train the next generation of experts in X-ray FEL science and related research areas. The curriculum includes a wide range of scientific and technical courses, workshops, and lectures, as well as soft-skills courses. The programme is supervised by the Ph.D. committee—composed of scientists, administrative staff, and experts in career development—which meets regularly to discuss the supervision and progress of the students. The programme is expected to become a crucial pillar in the development of strong in-house research activities, the foundation on which all successful user facilities grow and flourish.

Frequent exchanges via meetings, seminars, and other research networking initiatives lead to a strong sense of community and long-lasting identification with European XFEL. In 2022, students launched the European XFEL Ph.D. website, which is designed as a place for exchanging ideas and communicating activities for students inside and outside European XFEL.

The programme currently includes 45 Ph.D. candidates, with a diverse background of more than 15 different nationalities (Figures 1 and 2). Seven Ph.D. students graduated in 2022, and 13 more Ph.D. projects were approved.

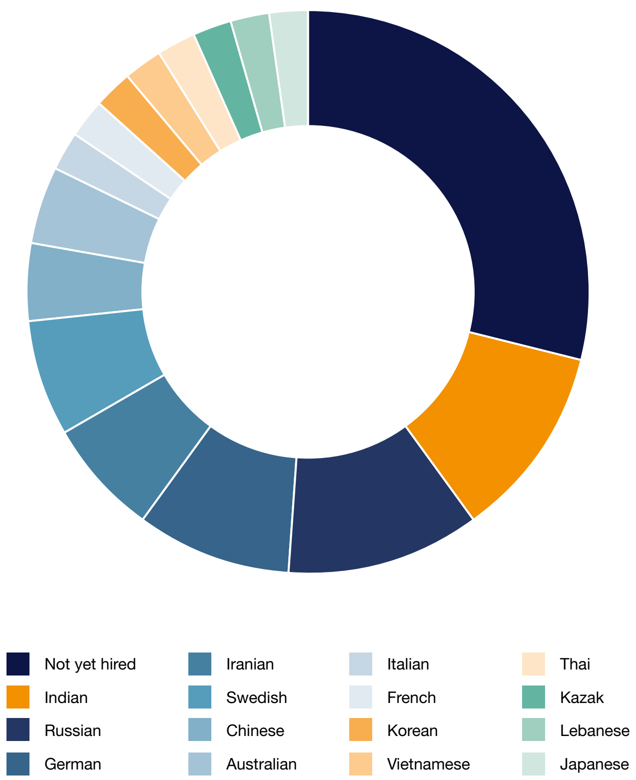


Figure 1: Nationalities of Ph.D. students at European XFEL

Figure 2: Participants of the Students' and Science Days 2022, including the European XFEL Ph.D. students

Figure 3: Students' and Science Days 2022

In line with similar research institutions, the gender distribution at European XFEL is rather unbalanced among scientists, engineers, and technicians. To improve this situation, European XFEL is committed to actively supporting the careers of female colleagues and to increasing the number of women in STEM disciplines. In accordance with the European XFEL Gender Equality and Diversity Plan (GEDP), this includes attracting more female students to the Ph.D. programme (Figure 3).

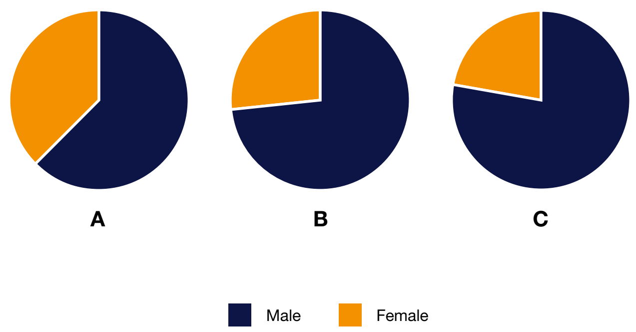


Figure 4: Gender balance of Ph.D. students at European XFEL: A) first year, B) second year, and C) third+ year

An important objective is the expansion of the European XFEL user community through new scientific collaborations with the shareholder countries. This is promoted by shared Ph.D. student projects, which are co-financed by European XFEL and universities in shareholder countries. To date, eight shared Ph.D. students are affiliated with six universities outside Germany. Collaboration agreements with other universities of shareholder countries are in preparation.

The annual three-day European XFEL Students' and Science Days (SSD) provide a platform for facility-wide exchange on internal research activities. The first day is fully organized and managed by the Ph.D. students. At the SSD, students are encouraged to present their own research to the scientific and technical staff at European XFEL and to discuss the research done by their peers and more senior researchers. With over 100 participants, the 2022 SSD was the first fully in-person event, very much appreciated by the early-career staff (Figure 4).

In 2022, in-person activities included a monthly Ph.D. seminar, the SSD, and other social events. Increasing onsite activities has strongly facilitated connections among the students, enhancing the visibility of their individual projects, while at the same time encouraging interdisciplinary cooperation and providing a spotlight for the diversity of the Ph.D. programme.

BUDGET AND THIRD-PARTY FUNDING

At the end of 2022, 98.7% of the European XFEL construction budget was spent. The annual operation budget was 140.7 million euro (M€) in 2022 and will increase to 145.7 M€ in 2023.

Parallel to spending from the annual operation budget, investments from the remaining construction budget continued in order to finalize some SASE installations—such as a third instrument port at the beamlines and an undulator for circular polarization—as well as to prepare for construction of the new office building and visitor centre.

In 2022, European XFEL could fully exploit new financial planning options to prepare for future big investments by creating an “indicative” budget through the pre-allocation of operation funds. The indicative budget is reported as part of the Facility Development Programme (FaDeP), describing and showing the planned expenses and their relation to the future-oriented development of the facility, including strategic activities and contingency plans. The FaDeP has helped increase the transparency of financial reporting and provided some flexibility for financing bigger projects currently in a pilot phase. It will also guarantee financial certainty in times when the geopolitical situation is uncertain.

The overall construction budget of European XFEL amounts to around 1.25 billion euro (2005 value). Forty-six percent 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.

The total European XFEL payment budget in 2022 amounted to 152 M€. Of this, 141 M€ (93%) was related to operation and 11 M€ (7%) was allocated to ongoing construction projects.

Recurrent and capital costs were the largest parts of the costs, totalling 78 M€ (51%). Another 69 M€ was spent on personnel, including staff from DESY. A further 5 M€ was allocated for smaller upgrades.

For 2023, an increased annual payment operation budget of 145.7 M€ was approved by the European XFEL Council, with a further 11.2 M€ being approved for finalizing the construction phase budget.

Besides the core funding by the shareholder countries, third-party funding plays an important role within the budget portfolio of European XFEL, providing flexibility for important projects. The European Union (EU)—within the framework of its Horizon 2020 and Horizon Europe research and innovation programmes—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 2022, European XFEL participated in 16 research projects, nine of which were funded by the EU Horizon 2020 and Interreg programmes, and eight by national funding organizations, such as DFG and the German Federal Ministry of Education and Research (BMBF).

The overall income from these projects was 1.0 M€, of which 80% came from European and international funding and 20% from national funding. The funds spent by third-party projects amounted to about 1.1 M€ in 2020 and 1.3 M€ in 2021 and 2022.

In 2022, five staff members were employed exclusively for third-party–funded projects. Two of these projects ended, and six new projects were started.

Budget 2022

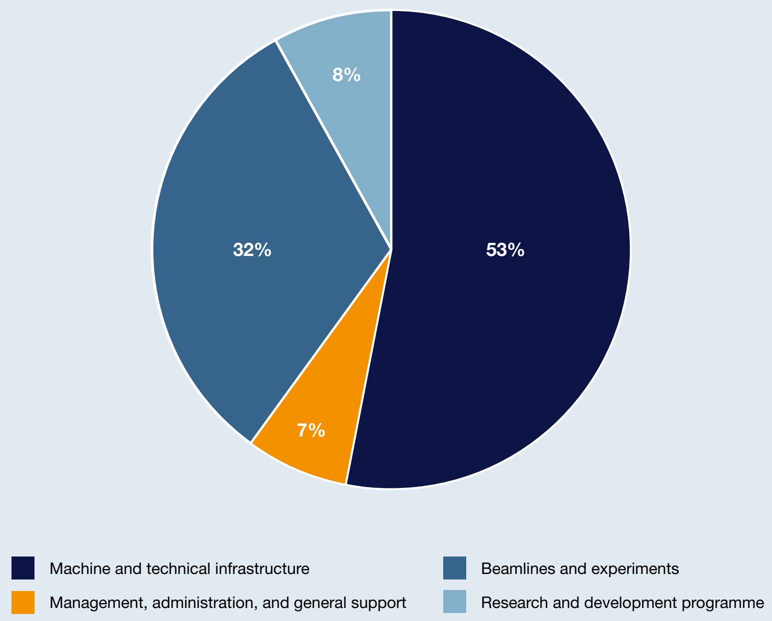


Figure 1: Payments by major activity in 2022

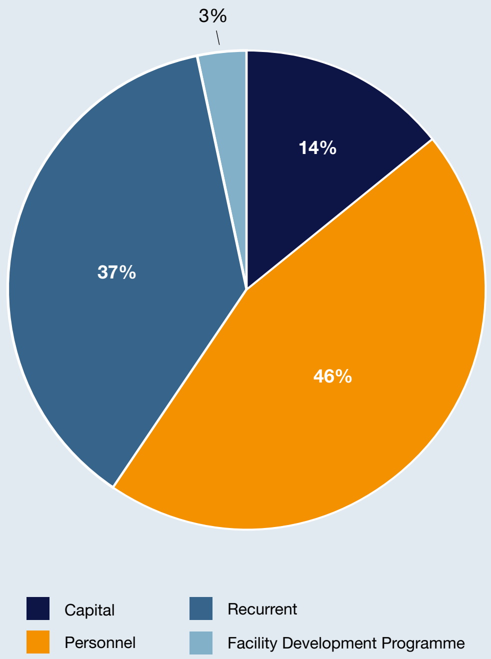


Figure 2: Payments by budget items in 2022

MANAGING QUALITY, SAFETY, RISK, AND CUSTOMS

Quality management

In 2022, overall improvements in quality management—comprising different quality-oriented services, procedures, and guidelines—resulted in tangible enhancements to processes and procedures. In addition, new areas were identified on which European XFEL needs to focus in the coming years. The optimization potential and adjustments are mostly connected to the maturing of the European XFEL as a facility as well as to some changes in the legal framework the company has to follow.

Due to the geopolitical situation and high inflation, special focus was put on adjusting the budget planning processes and ensuring the long-term financial stability of the company, using different planning tools and processes.

In addition, to cope with the disproportional rise in costs for energy consumption, the process of buying electrical power was adjusted. Although European XFEL has developed a procurement strategy for this volatile market in close collaboration with DESY and qualified external consultants, closer coordination with DESY and intensive observation of the market were necessary. To ensure the best possible prices, the procurement is done in up to 12 tranches per year and, where possible, well in advance. This process minimizes the risk of procuring power at times when prices are high and keeps a large degree of flexibility. Although this concept worked quite well in the last few years, 2022 brought new challenges. The significant price increase for electricity was difficult for European XFEL to pay, and potential saving strategies to reduce power consumption had to be developed. Thanks to close collaboration with DESY, these difficulties could be managed and strategies developed effectively. However, areas for improvement became apparent and can now be better addressed.

Environmental sustainability is an area of development on which European XFEL needs to focus. For example, only renewable energy will be used at European XFEL from 2023 onwards. This change will reduce the company's CO_2 emissions by 15 000 t per year. The heat derived from cooling down the facility's accelerator is currently used to heat buildings at DESY, with ongoing considerations to also use it for central heat supply in nearby residential quarters. In addition, by combining different measures, a 44.6% reduction in European XFEL's heat energy consumption was achieved (even with additional buildings) compared to 2019. These examples show that sustainability strategies can be used to successfully accelerate the development and adjustment of quality management processes, while having a big impact on the facility itself. The global climate crisis, the growing emphasis on corporate sustainability, the rapid growth of so-called "cleantech", and the increasing interest among stakeholders and shareholders will make environmental sustainability a management priority in the coming years.

The European quality management activities—supported by regular internal audits and an external end-of-year audit—aim to combine the state-of-the-art quality management of international scientific institutions and research infrastructures with modern insights into the administration of large service units, especially with regard to safety and reliability requirements. The activities established and the procedures implemented or adapted in 2022 were examined in the light of various quality aspects: 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 the European XFEL shareholder countries and the legal boundary conditions for administrative processes were addressed.

Table 1:

Number of work accidents during each quarter of 2022. Declared accidents are those resulting in an absence of more than three working days. All other accidents are considered minor. Commuting accidents are also included in the minor or declared column.

Quarter	Minor	Declared	Total
Q1	2	3	5
Q2	2	6	8
Q3	4	2	6
Q4	3	2	5
Total	**11**	**13**	**24**

Enterprise resource planning system

To improve and extend the services offered by the administrative groups and increase efficiency in administrative processes, European XFEL implemented an enterprise resource planning (ERP) system in 2022.

By storing and managing data from every stage of administration, the ERP system reduces errors that originate from working with potentially deviating data from different sources and guarantees the long-term quality assurance of financial and facility data. It integrates, standardizes, and, to a significant extent, automates different administrative tasks from procurement, finance, controlling, logistics, and warehousing, thereby improving the reliability, transparency, and productivity of administrative processes.

In 2015, with the support of external consultants, European XFEL started to systematically analyse its administrative processes and to collect requirements for an ERP software solution. Based on these requirements, the company conducted a public tender for procurement of the ERP system. In January 2018, Infor (Deutschland) GmbH was commissioned to implement the ERP system at European XFEL. The migration from other systems was successfully completed, and the ERP system went live in May 2022. Although it has been in full swing ever since and many improvements are already visible, during the first months of operation, further optimizations were identified, which will be implemented by mid-2023.

To ensure reliable operation and continuous improvement of the ERP system and connected processes, an integrative team was formed, consisting of members from administrative groups and the IT group.

Within the "HR 2.0 – Next Generation HR IT" project, which was launched in 2021, another ERP module will be added in 2023 to significantly optimize and simplify personnel and working-time–related processes.

Procurement

After the successful introduction of the ERP system, the digitalization of the procurement process continues to progress. Additional electronic catalogues have been and will be connected for the automated ordering of standard items. This enables process optimization and reduces administrative workload for the requester, the Procurement group, and the Finance group.

In addition, preparations are under way to implement stock items at the warehouse and manage the process in the ERP system. This digitalization will enable quick and easy availability of the most commonly used items and spare parts. The environmental footprint will be improved by reducing external packaging and fuel used in transport throughout the supply chain.

Safety

In 2022, the number of work accidents increased again compared to the previous two years, but, compared to the years before the pandemic, the numbers are still relatively low. There were no accidents in 2022 leading to long-term effects. In total, 24 accidents were reported, of which 11 were considered minor, leading to an absence of three or less working days. The other 13 so-called “declared accidents” resulted in absences of more than 3 working days. Out of the 24 reported cases, including minor and declared “accidents”, 9 were commuting accidents.

Instruction about workplace risks is one of the key responsibilities of European XFEL towards its employees, users, and guests. The content and style of the corresponding online training modules were revised. In addition, new videos and voluntary training modules were implemented, for example on so-called “dead-man switches”, “oxygen-deficiency” sensors, and fire alarms.

Dead-man switches were introduced in the lab area of the headquarters building (XHQ) to facilitate staff members working alone. These devices automatically inform the technical emergency team (which is on site 24/7) if someone working alone does not move for a specified time.

A project for machine safety and required technical documentation also started in 2022, with the goal to implement CE compliance for equipment and machines at European XFEL (Figure 1).

A laser safety review took place in summer 2022, and, as a result, a laser safety committee involving several parties was established. One of its main goals is a regular, active exchange of knowledge on laser safety matters between experts in the field across the company.

Radiation protection

In 2022, a third instrument, SXP, started operation at the SASE3 soft X-ray FEL source. The joint radiation protection organization of European XFEL and DESY collaborated with many groups at both institutions to implement and install the SXP radiation protection personnel interlock system and the safety equipment protection system in a short time. European XFEL supplied the beam shutter and installed it, while DESY provided the PANDORA detectors for radiation measurements, the burn-through monitors, the air boxes, and the hutch monitors, in addition to organizing and conducting the technical inspection (TÜV) tests of the personnel interlock system. European XFEL supplied the active instrument beam stop (AIBS) devices, which were manufactured at DESY, as well as the safety equipment protection system interlocks, and contributed to documentation for the TÜV tests. DESY was responsible for the entire implementation of the personnel interlock system. Altogether, this joint effort was one of the contributions that enabled the SXP instrument to successfully receive first beam in October 2022.

Risk management

In 2022, processes for well-synchronized risk management (RM) and asset management (AM) were successfully implemented at European XFEL. For the first time, the full cycle of a risk reporting period was conducted together with the Asset Management group, with RM and AM being synchronized to exploit the synergies of the two fields.

The administrative groups were successfully integrated into the corporate RM process. The RM process for projects running in parallel with the operation of the facility was set up and implemented.

At the same time, a third AM report was completed. It includes the group-specific AM strategies and a company-wide requirements analysis that brought together all the different AM approaches.

Customs and export control

European XFEL secures all processes that may be affected by export control and, at the same time, strives to significantly improve the quality of all customs-related processes (import and export of goods as well as technical support). All national, EU, and US regulations are considered in their most current version. The immediate benefits include faster processing of all import and export procedures, which is particularly important for the timely arrival of samples and equipment for experiments, safe shipping of high-quality equipment abroad for repair or experiments, and, wherever possible, reducing or even avoiding import costs, such as customs duties and import taxes.

In 2022, special emphasis was put on implementing a dual-use policy and improving direct user support. Other improvements include the simultaneous checking of all proposals for import bans as well as for regulations for incoming samples (e.g. veterinary inspections) and equipment temporarily imported for the experiments in order to properly define import procedures. In addition, procedures are coordinated with users well ahead of time to save import duties and protect against delays, rejection, or confiscation during import.

Figure 1:

Instruction of staff members about safety documentation for machines

INTERNATIONAL COLLABORATION

After two years of pandemic-related travel restrictions, European XFEL permitted regular face-to-face visits in 2022 again, enabling staff members to engage more personally with collaboration partners. Such travel mainly centred on attending meetings and schools in the shareholder countries. These included the DanScatt Annual Meeting in Copenhagen in August, the 15th International School and Symposium on Synchrotron Radiation in Natural Science in Przegorzały, Poland, in August, and the 7th School of XFEL and Synchrotron Radiation Users in Liptovský Ján, Slovakia, in November. These meetings were important platforms for getting to know and inspiring the current and future generations of scientists and users. In March, European XFEL contributed to the annual "HERCULES European School: Neutrons and Synchrotron Radiation for Science" and welcomed 16 students for a two-day visit to European XFEL (Figure 1). Staff members also reached out to potential new collaboration partners in both academia and industry, in particular in the shareholder countries, to establish new connections and co-development projects there.

European XFEL and DESY helped to co-found the Scienziati Italiani in Germania Network (SIGN) to encourage interactions between scientists in Italy and Germany (Figure 2). The initiative provides a network for Italian scientists working in Germany. European XFEL Scientific Director Sakura Pascarelli now serves as Deputy Director of SIGN.

Despite the slowly easing COVID-19 situation, the 2022 European XFEL Users' Meeting was still held remotely. The same was true for the 14th International Conference on Synchrotron Radiation Instrumentation (SRI2021), which—after having been postponed from 2021—was held in 2022 as an online meeting, enabling 1160 participants from around the world to meet virtually.

Within the two European Framework Programmes Horizon 2020 and Horizon Europe as well as the Interreg programme and the Röntgen Ångström Cluster (BMBF), European XFEL is involved in multiple projects (Figure 3).

Figure 1: Students of the HERCULES European School visiting European XFEL

Figure 2: Co-signatories of SIGN at the inauguration ceremony

Figure 3: Collaborative third-party-funded projects with the partners of European XFEL

Figure 4: Attendees of the MHz TOMOSCOPY kick-off-meeting

Also, Patrik Vagovic, a scientist working at CFEL at DESY and SPB/SFX at European XFEL, was awarded one of the first European Innovation Council Pathfinder grants of 3.15 million euro (M€) for his MHz TOMOSCOPY project by Horizon Europe, for which European XFEL will receive 0.81 M€ over 3.5 years (Figure 4).

The Photon and Neutron Open Science Cloud (PaNOSC) project ended in November 2022. The main goal of PaNOSC was to establish FAIR—findable, accessible, interoperable, and reusable—data procedures, tools, and services at six European research infrastructures, covering all aspects from data policy recommendations to software development. Outcomes of PaNOSC were registered with the European Open Science Cloud (EOSC) so users could find the developed services there and benefit from them more readily.

In the framework of the Röntgen–Ångström Cluster, the X-ray based drug design platform (XDD) project, led by European XFEL, started in April with the University of Gothenburg, AstraZeneca, MAX IV, DESY, and Universität Hamburg. The consortium is developing a new structure-based drug design platform by exploiting the potential of X-ray FEL sources for drug discovery projects for future treatment of COVID-19 and the neglected tropical disease lymphatic filariasis.

European XFEL also continued to collaborate with researchers from Hamburg and southwestern Scandinavia—including research facilities such as MAX IV, ESS, DESY, and EMBL Hamburg—to promote life science innovation and research as part of the Hanseatic League of Science (HALOS) project fostered within the European Regional Development Fund Interreg Öresund–Kattegatt–Skagerak (ÖKS) programme.

European XFEL is active in the League of European Accelerator-based Photon Sources (LEAPS) consortium, a network of European facilities that work closely together to promote joint initiatives between member institutes. The Horizon 2020 project LEAPS-INNOV (GA No. 101004728) was aimed at developing technological and research capabilities between LEAPS members and industry partners. European XFEL scientists also participated in the biannual scientific LEAPS conference, titled “LEAPS Meets Quantum Technology”, in Elba, Italy, to strengthen Europe’s leading role in science and innovation. A major topic of the conference was to identify how X-ray sources such as the European XFEL could be used to address science and technology questions in quantum technology. This was the first of a series of conferences bringing together LEAPS and the scientific community.

The European XFEL management continued to collaborate with the European Commission, welcoming Apostolia Karamali and Agnes Robin from the Unit for R&I Actors and Research Careers (Figure 5). The LEAPS-initiated visit to the European XFEL and DESY facilitated discussions about the role of research infrastructure in partnerships such as LEAPS and beyond. The European XFEL management also participated in a meeting with Maria Leptin, President of the European Research Council (ERC), at DESY in June.

European XFEL has been one of the eight international research facilities in the EIROforum partnership since 2010. EIROforum is a valued platform for regular exchange between institutions, including joint events. In 2022, the EIROforum workshop “Grand Challenges in AI and Data Science”—which covered everything from data acquisition to data mining—was organized as a hybrid event at EMBL in Heidelberg, Germany, bringing together experts from all EIROforum member institutes and beyond.

Within the FELs OF EUROPE collaboration, European XFEL has also taken an active role, and European XFEL Scientific Director Serguei Molodtsov has continued to serve as Chairman. The collaboration provides a platform for exchange between the different facilities as well as regular tutorials and workshops organized by its members. In addition, the annual international Science@FELs 2022 conference took place at DESY and European XFEL in September (Figure 6).

European XFEL also welcomes the opportunity to widen its current collaboration and user network, including both academic and industry partners. Such an opportunity arose at the Big Science Business Forum (BSBF) 2022, taking place in Granada in October, which allowed European XFEL staff members to tighten long-standing collaborations and start discussions with potential new partners.

The year 2022 was proclaimed the International Year of Basic Sciences for Sustainable Development (IYBSSD2022). European XFEL joined the initiative to raise awareness that flourishing basic science and research are crucial for sustainable development.

Figure 6: Participants of the Science@FELs 2022 conference

Figure 5: Apostolia Karamali, Head of Unit ERA & Innovation of the European Commission, visiting the SPB/SFX instrument

CONTACTS TO INDUSTRY

Figure 1: Visitors at the National ILO meeting tour the experiment hall

Figure 2, top:
Members of the ILO participate in the hybrid National ILO meeting

Figure 3, left:
Bilateral meeting with the Slovak Investment and Trade Development Agency at the Slovak Industry Vision Day 2022

To promote industrial collaborations with European XFEL, the Industrial Liaison Office (ILO) supported the organization of the Big Science Business Forum 2022, which took place in October in Granada, Spain. The event brought together key suppliers and high-level representatives of various international science institutes and laboratories, including European XFEL, to explore new possibilities for advancing the development of novel technologies. This included presentations of experts from European XFEL and two dedicated booths for both European XFEL and the League of European Accelerator-based Photon Sources (LEAPS), increasing the chances of co-development with industry for key cutting-edge technologies.

European XFEL also participated in the Slovak Industry Vision Day on 24 November, creating connections to new technology providers in the Visegrád Four countries.

European XFEL has facilitated research in applied science of industrial interest in structural biology by involving pharmaceutical companies. A pilot collaborative experiment using the European XFEL was successfully conducted with an international biopharmaceutical company, Sosei Heptares. The experiment demonstrated a powerful approach to determining three-dimensional structures of biomolecules with atomic resolution. The collaboration used the European XFEL’s SPB/SFX instrument to investigate G protein-coupled receptor (GPCR) crystals generated by Sosei Heptares in order to provide insights for drug discovery and design.

OUTREACH

Figure 1:
Students from the University of Strasbourg in France tour the experiment hall.

Figure 2:
Experimenting with a microscope at the YoTa holiday event

Visitor tours

After a long period of only virtual tours due to the COVID-19 pandemic, European XFEL was finally able to resume guided visitor tours on the research campus in March 2022. Around 1200 visitors took part in 47 guided tours during the rest of the year. Due to high demand and limited capacity, students and young scientists were given priority.

New videos

European XFEL's communication and events were supported by 28 new videos, 20 of which were produced in-house, on topics such as new scientific developments, user portraits, and the European XFEL company values.

Outreach for schools

As part of this year's "Physik im Advent" competition, which is organized annually by the University of Göttingen, 22 winners from Gymnasium Oberalster in Hamburg visited European XFEL. The students received a short introduction to the facility, complemented by a guided tour of the experiment hall, before taking part in practical science demonstrations.

Fifteen participants of the regular holiday event for Young Talents Hamburg (YoTa) also spent a day on site learning about research with X-rays at European XFEL before diving into experiments. Half of the group was taught how to construct a microscope at the dry sample preparation lab, while the other half was busy programming a robot.

Outreach for the general public

At the annual science festival "Highlights der Physik" in Regensburg, representatives from European XFEL presented posters, exhibits, and a video programme. Over 40 000 visitors attended the six-day programme either on site or online.

In July, the city of Schenefeld celebrated its 50th anniversary with a public event on the market square in the centre of Schenefeld. The festival offered numerous hands-on activities. At the European XFEL booth, visitors could see, feel, and taste fascinating science in action: Ice cream frozen within minutes by liquid nitrogen was

Figure 3:
More than 40 000 people visited the "Highlights der Physik" exhibition in Regensburg.

Figure 4:
Ice cream frozen with liquid nitrogen at the 50th anniversary of the city of Schenefeld

handed out in different flavours; diffraction pattern selfies could be taken as a souvenir; and, in a DIY X-ray chamber, children could take a guess what was inside their Kinder surprise egg before eating it. A highlight was European XFEL Managing Director Nicole Elleuche and Senior Scientist Joachim Schulz dressing up as superhero Flash and sidekick Doc Brown from the film "Back to the Future" to explain the "super powers" of the European XFEL on stage.

European XFEL returned for the city of Schenefeld's annual Christmas market, where the company presented posters and informational material. At a science quiz, visitors could test their knowledge about the facility and its science.

Lighthouse—European XFEL visitor and conference centre

In November 2022, earthworks began for the new European XFEL visitor and conference centre, due to open in 2024. Its name, Lighthouse, was chosen from suggestions by European XFEL staff. It refers to the X-ray laser as a beacon of research and is a tribute to the "light of the future" that it generates.

The two-storey visitor centre will offer 350 m² of space for a permanent exhibition, for which planning continued in 2022. In addition, the building will offer 200 m² for special exhibitions, an area for virtual-reality applications, the Xcool Lab with two student laboratories, and rooms for conferences and events.

The construction costs for the Lighthouse will amount to 15 million euro (M€). The German federal state of Schleswig-Holstein is supporting the project with 2 M€ and providing a teaching position for the operation of the Xcool Lab from summer 2023 onward.

The permanent exhibition will explain in English and German how the X-ray laser works and what insights it can contribute to solving major societal challenges. At the centre of the exhibition will be a model of the facility, around which other interactive exhibits will be grouped. These will include hands-on science experiments, original objects such as an accelerator cavity, and computer-based activities including a game that simulates conducting an experiment at a scientific instrument. In 2022, the tender was awarded for the production of the exhibition, which will be installed in the building in early 2024 after various planning and production work packages are completed in 2023.

Planning also continued for the Xcool Lab, a practical initiative that will help motivate young people to enter careers in science, technology, engineering, and math (STEM). The two student laboratories for physics and biochemistry are designed for junior and senior high school students to conduct hands-on curriculum-linked experiments and gain insight into scientific research. In 2022, work began on the first experiment modules, which focus on the physics of X-rays and virus research. The modules will be piloted to local school classes in German and later made available in English.

DIRECTOR'S OUTLOOK

Looking to the future has become difficult in recent years, first with the pandemic and then with the Russian invasion of Ukraine. Although significant progress has been made in the development of the European XFEL, the last three years have also been a period of constant crisis management. With the war in Ukraine continuing, we expect that 2023 will prove to be another challenging year for our international facility.

There are, however, many things to be optimistic about. The European XFEL is getting closer to its full operational capacity, and we expect to deliver an even more exciting science programme to the benefit of our user community. In the past years, we have achieved tremendous improvement in the stability and quality of the operation of the facility. In particular, I am looking forward to further improvements to the superconductor accelerator, where in 2022 one of the cold compressors was retrofitted with magnetic bearings instead of ceramic bearings. If successful, the other three cold compressors will be retrofitted in 2023. This upgrade should then significantly reduce cryo-failures, which typically bring the facility and operation down for at least 36 hours, with considerable impact on experiments. The improvements are expected to be another big step forward for accelerator operation.

Importantly, 2023 will be the year in which we will finalize our strategy. The work on this project has been intense and is now resulting in a fully formed picture, with a particular focus on the importance of the facility's successful operation in this decade. Our revised scientific strategy will include shifting from proof-of-concept experiments conducted in the startup phase during the facility's first years towards science-based experiments driven by important societal challenges. I am convinced that the European XFEL, with its unique capabilities, can make significant scientific contributions to address health issues, sustainability, digitalization, and climate change. To ensure a successful transition, we will need to actively engage with our present and future user community, while simultaneously continuing mid-term developments to keep European XFEL at the forefront of X-ray FEL science. This includes delivering an attosecond science programme and opening new science areas by pushing our photon energies higher and higher, accessing lasing above 50 keV in the next decade through the development of superconducting undulators.

Having reviewed four out of our six original instruments, with a seventh in commissioning, we have a strong basis for developing our instrument portfolio in the coming years. We also plan to attract funding for new instrumentation and beam transport to build two new beamlines for four instruments in the two still-empty tunnels leading to the experiment hall. We will, in parallel, continue to work with DESY on the development of the superconducting accelerator towards a facility with increased capacity and new capabilities by the mid-2030s.

Despite the challenges of 2022 and any obstacles the future may hold, I am certain that 2023 will be an exciting year for our facility, consolidating the user programme while pointing to the future.

Robert Feidenhans'l

FACTS AND FIGURES

European XFEL staff outside the company restaurant, BeamStop

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 ultra-short 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. The campus also has a warehouse and workshop building (completed in 2018), a company restaurant, BeamStop (completed in 2019), a guest house (completed in 2021), and an undulator hall (completed in 2021). A second office building is due to open on the campus in 2023 and a visitor and conference centre, Lighthouse, in 2024.

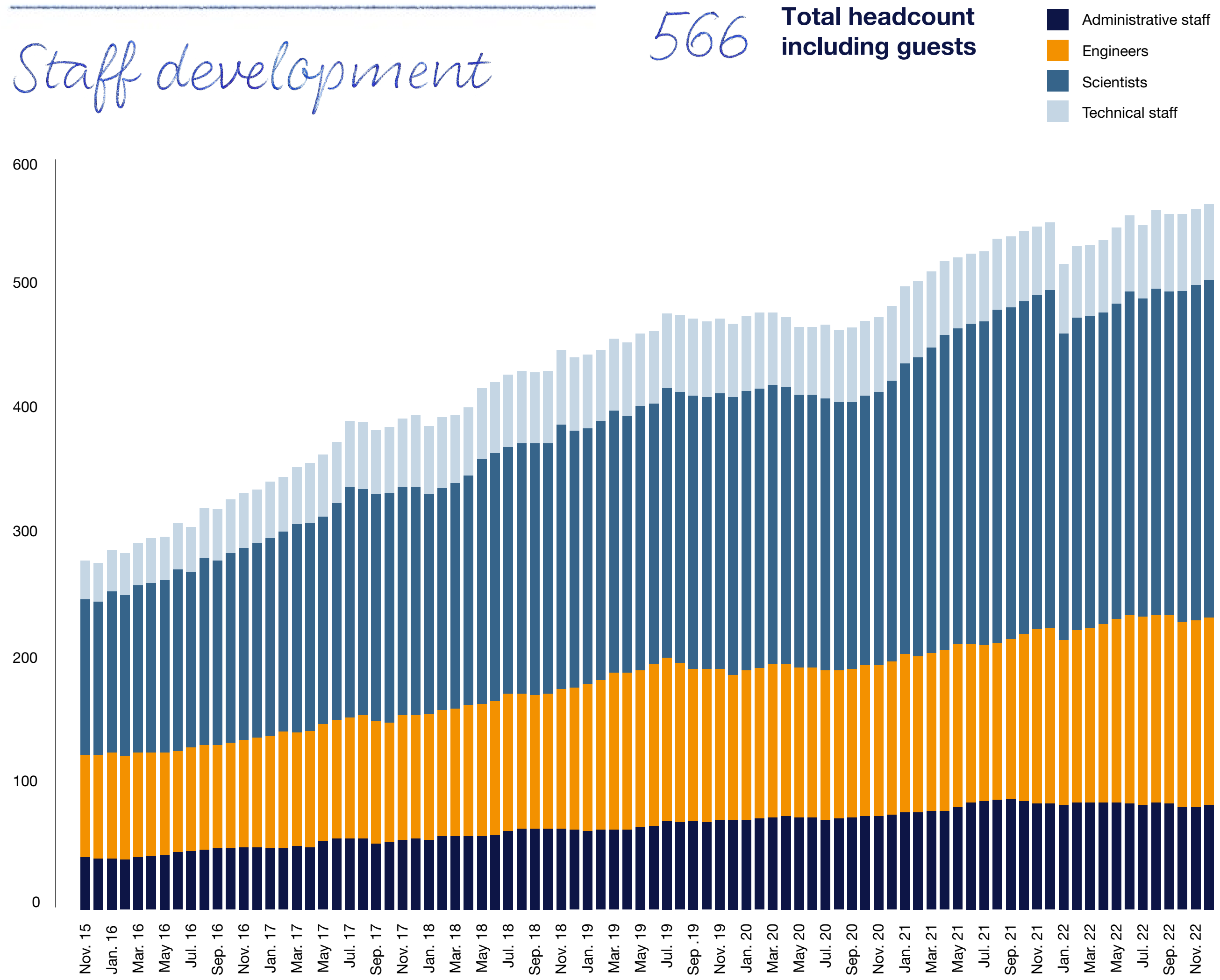
As of December 2022, 12 partner countries are member states of European XFEL: Denmark, France, Germany, Hungary, Italy, Poland, Russia, Slovakia, Spain, Sweden, Switzerland, and the United Kingdom. The international partners have entrusted the construction and operation of the facility to the non-profit 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 operation budget for the facility is approximately 141 million euro. The construction costs, including commissioning, amounted to 1.25 billion euro (at 2005 price levels). In 2022, the host country, Germany (federal government, city–state of Hamburg, and state of Schleswig-Holstein) covered 58% of the costs. Russia contributed 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.

Figure 1: Aerial view of the European XFEL facility. Left to right: Schenefeld, Osdorfer Born, and DESY-Bahrenfeld sites.

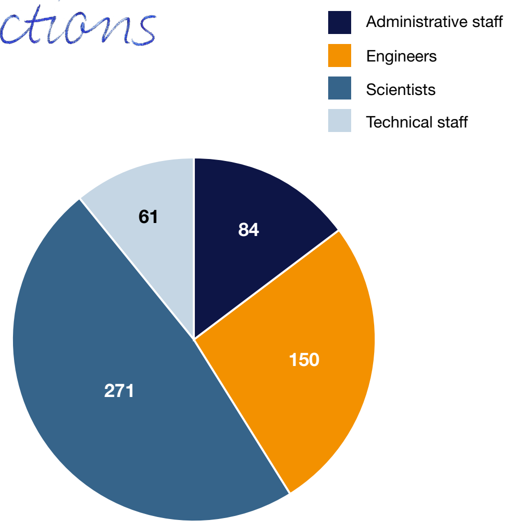
STAFF

Staff development

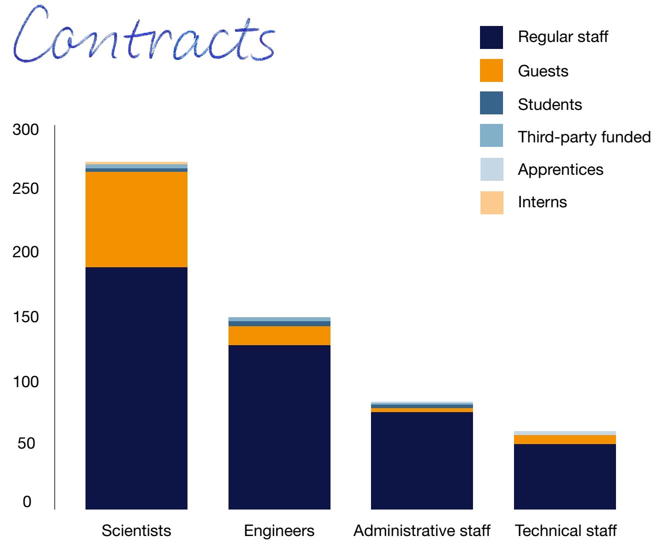
566 **Total headcount including guests**



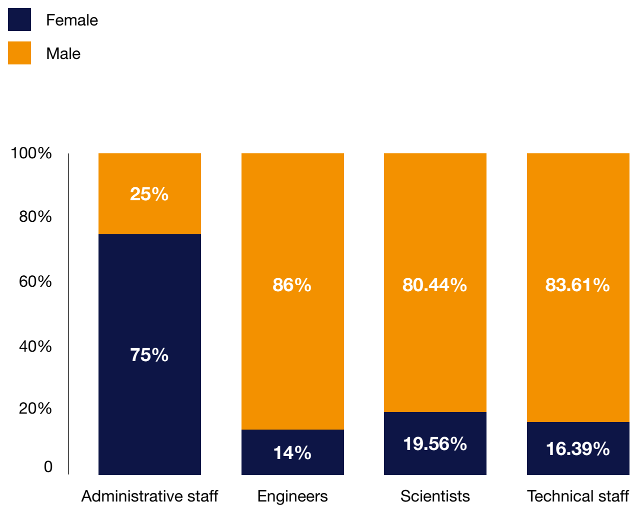
Functions



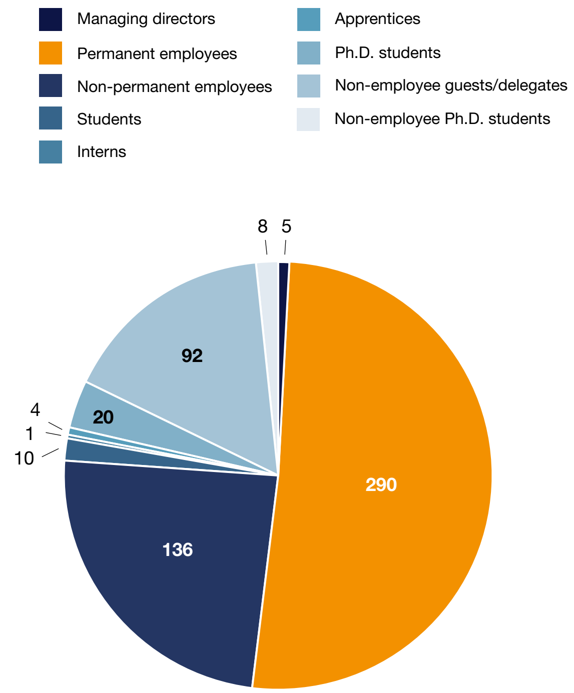
Contracts



Gender ratio

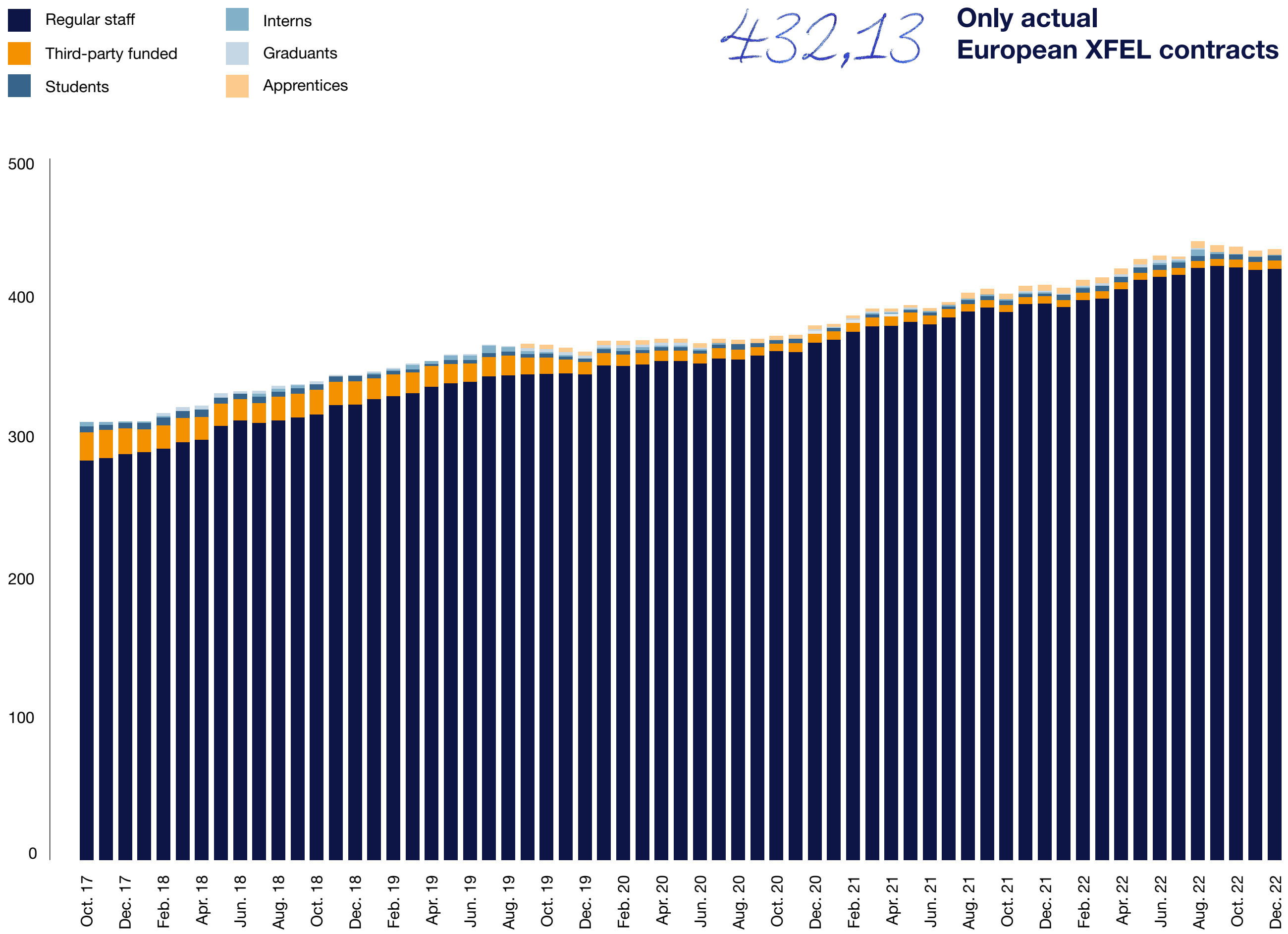


Contractual status



Full-time equivalents

432,13 **Only actual European XFEL contracts**

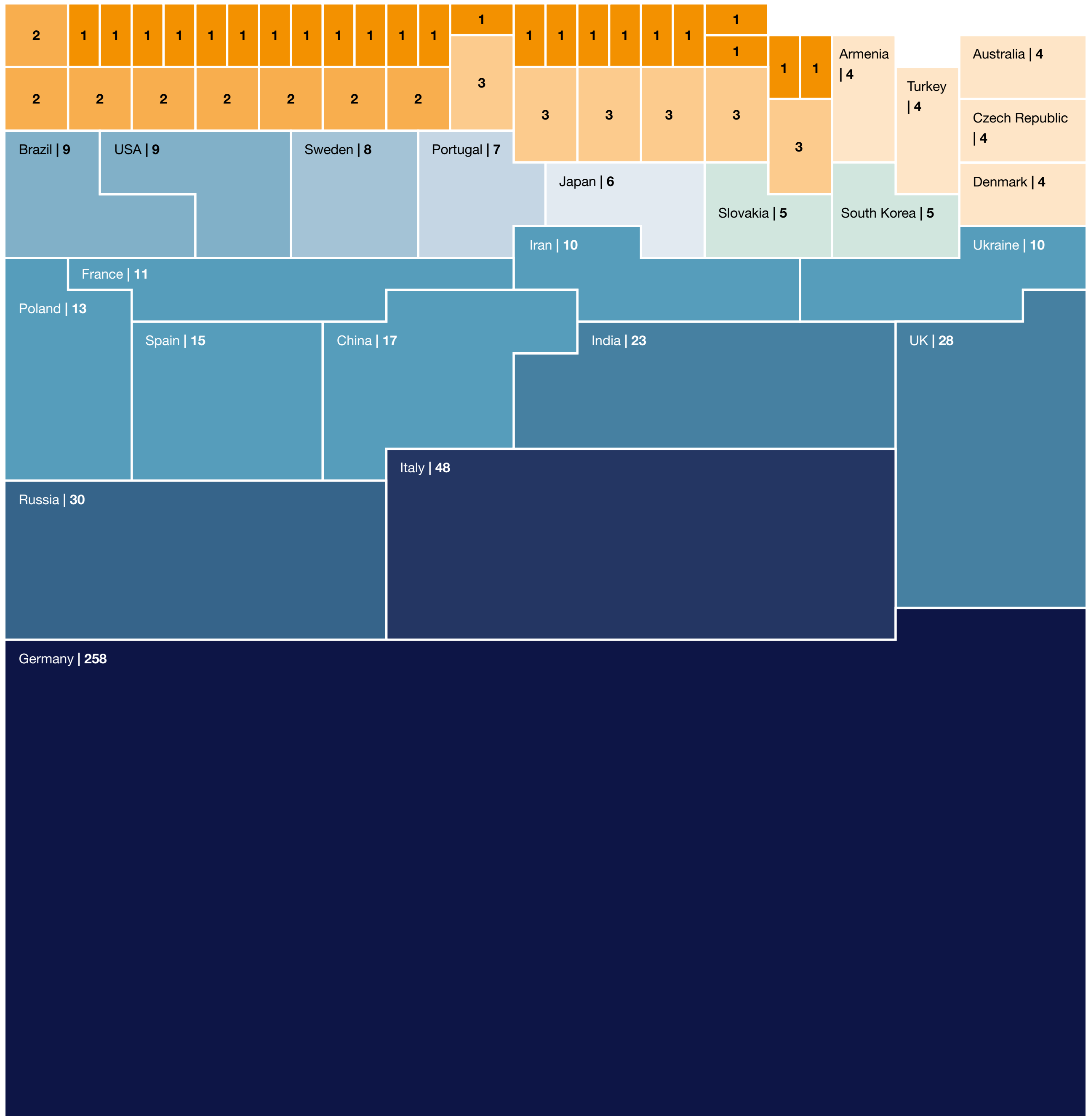


All Staff

60 Citizenships in total

23 Double citizenships

(1) Albania, Algeria, Arabian Republic of Syria, Austria, Azerbaijan, Bulgaria, Chile, Ecuador, Finland, Georgia, Ghana, Hungary, Kenya, Latvia, Lebanon, Malaysia, Philippines, Sudan, Thailand, The Netherlands, Venezuela, Vietnam, Yemen
(2) Canada, Indonesia, Jordan, Kazakhstan, New Zealand, Pakistan, Serbia, Switzerland
(3) Bangladesh, Croatia, Egypt, Greece, Mexico, Romania

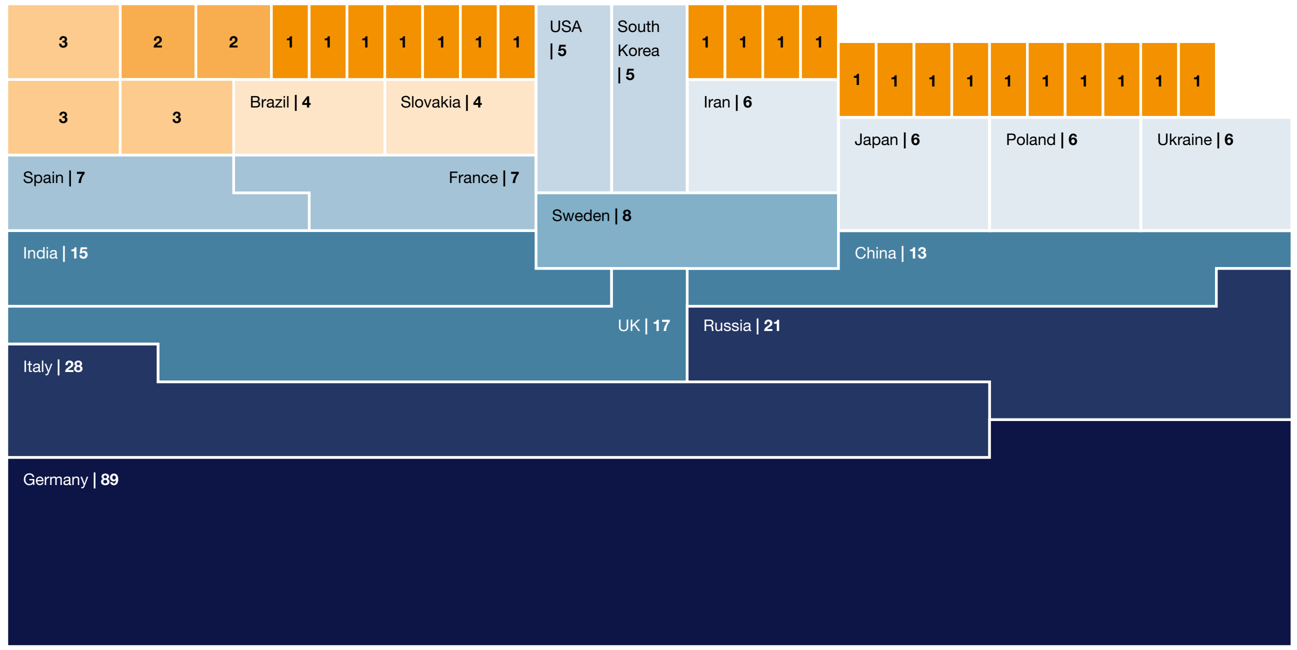


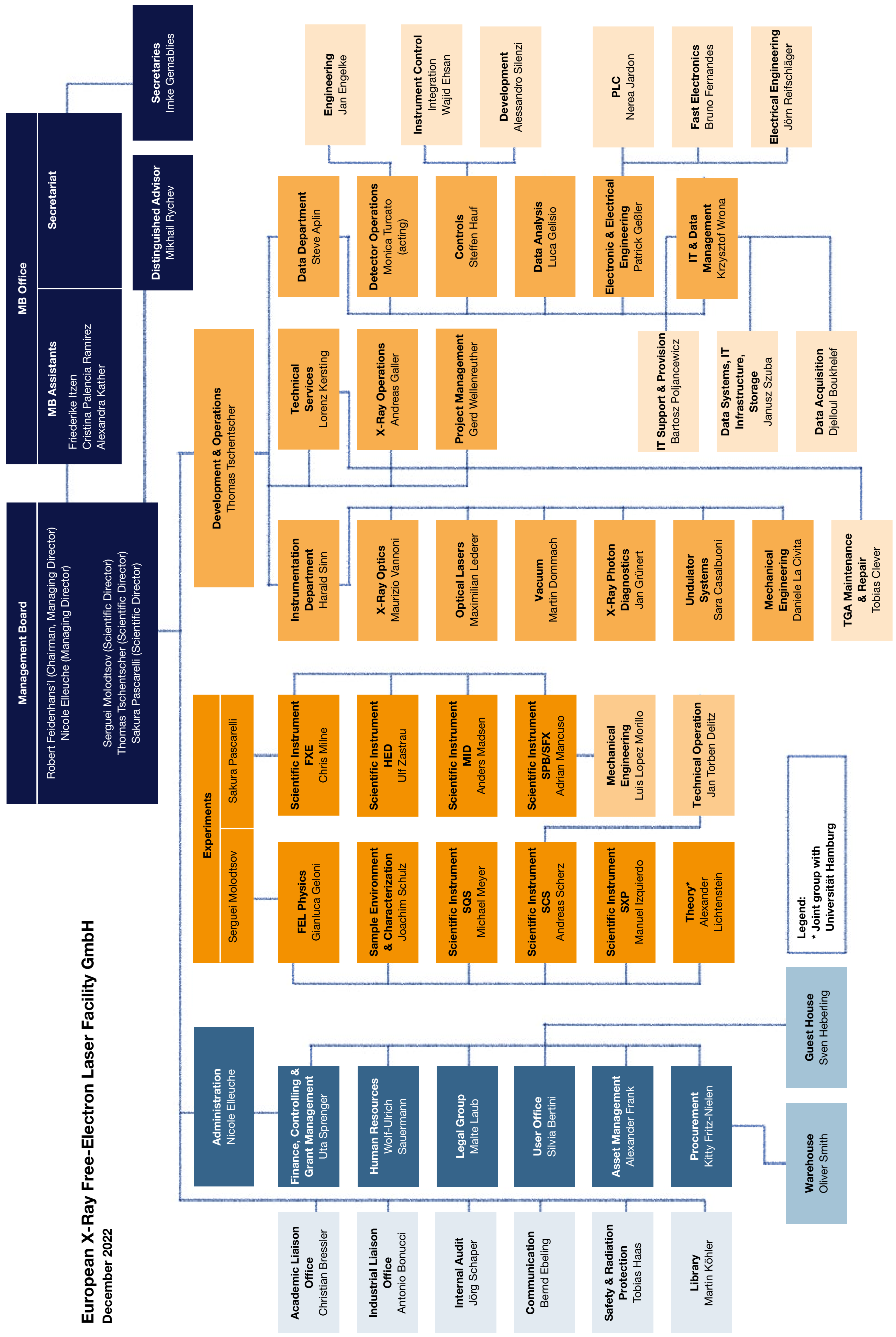
Scientific Staff

43 Citizenships in total

10 Double citizenships

(1) Algeria, Arabian Republic of Syria, Austria, Bulgaria, Canada, Chile, Georgia, Greece, Hungary, Indonesia, Jordan, Kazakhstan, Lebanon, New Zealand, Romania, Sudan, Switzerland, Thailand, Turkey, Vietnam, Yemen
(2) Australia, Egypt
(3) Czech Republic, Denmark, Portugal





SHAREHOLDERS

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

Member states	Present (bold) or 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)**

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. The Council meets at least twice a year. It functions as the shareholder assembly that decides important issues of company policy.

Chairperson		**Maria Faury** until 30 June 2022 (CEA, Paris) **Federico Boscherini** as of 1 July 2022 (University of Bologna)
Vice Chairperson		**Martin Meedom Nielsen** until 30 June 2022 (DTU, Kongens Lyngby) **James Naismith** as of 1 July 2022 (Rosalind Franklin Institute, Didcot)
Delegates	**DENMARK**	**Martin Meedom Nielsen** as of 1 July 2022 (DTU, Kongens Lyngby) **Morten Scharff** (DAFHES, Copenhagen)
	FRANCE	**Sylvain Ravy** (CNRS, Paris) **Marie-Hélène Mathon** until 30 June 2022 (CEA, Paris) **Maria Faury** as of 1 July 2022 (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	**Mikhail Kovalchuk** (NRC KI, Moscow) **Alexander Blagov / Mikhail Polyakov** (NRC KI, Moscow)
	SLOVAKIA	**Karel Saksl** (Institute of Materials Research, SAS, Košice) **Pavol Sovák** (P.J. Šafárik University, Košice)
	SWEDEN	**Lars Börjesson** until 15 September 2022 (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** until 30 June 2022 (Rosalind Franklin Institute, Didcot) **Jon Marangos** as of 1 July 2022 (Imperial College London)
Observers	**SPAIN**	**Guadalupe C. de Córdoba Lasunción** (Ministerio de Ciencia e Innovación, Madrid) **Rodolfo Miranda** (IMDEA Nanociencia / Universidad Autónoma de Madrid)
Secretary		**Malte Laub** (European XFEL, Schenefeld, Germany)
Vice Secretary		**Friederike Itzen** (European XFEL, Schenefeld, Germany)
Advisors	**FRANCE**	**Marie-Hélène Mathon** as of 1 July 2022 (CEA, Paris)
	GERMANY	**Christian Harringa / Wim Leemans** (DESY, Hamburg) **Andreas Zöller** as of 13 June 2022 (BMBF, Bonn)
	ITALY	**Federico Boscherini** until 30 June 2022 (University of Bologna) **Alberto Morgante** as of 1 July 2022 (University of Trieste and IOM-CNR, Trieste) **Daniele Sertore** (INFN, Milan)
	POLAND	**Zbigniew Gołębiewski** until 30 June 2022 (NCBJ, Otwock-Świerk) **Dagmara Milewska** as of 1 July 2022 (NCBJ, Otwock-Świerk) **Tomasz Leżański** (NCBJ, Otwock-Świerk)
	SLOVAKIA	**Martin Šponiar** (Ministry of Education, Science, Research and Sport, Bratislava)
	SWEDEN	**Lars Börjesson** as of 16 September 2022 (Chalmers University of Technology, Gothenburg) **Maja Hellsing** as of 16 September 2022 (VR, Stockholm)
	SWITZERLAND	**Doris Wohlfender-Bühler** (SERI, Bern)
	UNITED KINGDOM	**Rachel Reynolds** (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, all acting as proxy holders.

Chairperson and Managing Director	**Robert Feidenhans'l**
Scientific Directors and Proxy Holders	**Serguei Molodtsov** **Sakura Pascarelli** **Thomas Tschentscher**
Administrative and Managing Director	**Nicole Elleuche**

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		**Sabine Carl** (BMBF, Bonn, Germany)
Vice Chairperson		**Michał Wójtowicz** (NCBJ, Otwock-Świerk, Poland)
Delegates	DENMARK	**Morten Scharff** (DAFHES, Copenhagen)
	FRANCE	**Philippe Sassier** (CEA, Paris) **Stéphanie Dupuis-Lê Vàn** (DSFIM, Paris)
	GERMANY	**Christian Harringa** (DESY, Hamburg) **Konstantin Ott** until 31 March 2022 (BMBF, Bonn) **Andreas Zöller** as of 1 April 2022 (BMBF, Bonn)
	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) **Martin Šponiar** (Ministry of Education, Science, Research and Sport, Bratislava)
	SWEDEN	**Maja Hellsing** (VR, Stockholm)
	SWITZERLAND	**Peter Allenspach** (PSI, Villigen) **Doris Wohlfender-Bühler** (SERI, Bern)
	UNITED KINGDOM	**Rachel Reynolds** (STFC, 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 to the accelerator complex.

Chairperson	**Evgeny Levichev** from 24 October 2021 (BINP, Novosibirsk, Russia)
Members	**Evgeny Levichev** (BINP, Novosibirsk, Russia) **Franz-Josef Decker** (SLAC, Menlo Park, California, USA) **Luca Giannessi** (Elettra Sincrotrone Trieste, Italy) **Thomas Schilcher** (PSI, Villigen, Switzerland) **Catherine Madec** (CEA, Paris, France) **Andrzej Wolski** (University of Liverpool, UK) **Fernando Sannibale** (LBNL, Berkeley, California, USA) **Atoosa Mesek** (HZB, Berlin, Germany) **Nicolas Leclercq** (ESRF, Grenoble, France) **Sara Thorin** (MAX IV, Lund, Sweden)

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 buildup of the scientific capacity of the European XFEL facility, its full and effective utilization, and future developments required to maintain the scientific and technical productivity of the facility at the highest possible level.

Chairperson

Claudio Masciovecchio as of 21 November 2021 (Elettra Sincrotrone Trieste, Italy)

Members

Olga Alekseeva until 26 June 2022 (IC RAS, Moscow, Russia)
Guillaume Fiquet until 27 January 2022 (IMPMC, Paris, France)
Elspeth Garman (University of Oxford, UK)
Steve Johnson (ETH, Zürich, Switzerland)
Henrik Lemke (PSI, Villigen, Switzerland)
Anne l'Huillier (Lund University, Sweden)
Arwen Pearson (Universität Hamburg, Germany)
Alexander Popov (ESRF, Grenoble, France)
Philippe Wernet (Uppsala University, Sweden)
Robert W. Schoenlein (SLAC, Menlo Park, California, USA)
Nina Rohringer (DESY, Hamburg, Germany)
Ian Robinson (UCL, London, UK)
Jan Lüning as of 18 November 2021 (HZB, Berlin, Germany)
Tim Salditt as of 18 November 2021 (Georg-August-University Göttingen, Germany)
Paul Loubeyre as of 17 November 2022 (CEA/DIF, Arpajon, France)
Amina Taleb-Ibrahimi as of 17 November 2022 (CNRS - Synchrotron SOLEIL, Saint-Aubin, France)

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.

Chairwoman

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

Members

Branden Allen (Harvard College Observatory, Cambridge, Massachusetts, USA)
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)
Mark W. Tate (Cornell University, Ithaca, New York, USA)
Matthew Wing (UCL, London, UK)
Darren Spruce (MAX IV, Lund, Sweden)

Laser Advisory Committee

The Laser Advisory Committee (LAC) advises the European XFEL Management Board, the DESY Directorate, 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 directly 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)
Catherine Le Blanc (Laboratoire LULI, Ecole Polytechnique, France)
Emma Springate (STFC Rutherford Appleton Laboratory, Didcot, UK)
Clara Saraceno as of February 2022 (Ruhr University Bochum, Germany)

Secretaries

Nele Müller until 30 June 2022 (DESY, Hamburg, Germany)
Jörg Hallmann (European XFEL, Schenefeld, Germany)
Karolin Baev as of 1 July 2022 (DESY, Hamburg, Germany)

Proposal Review Panels

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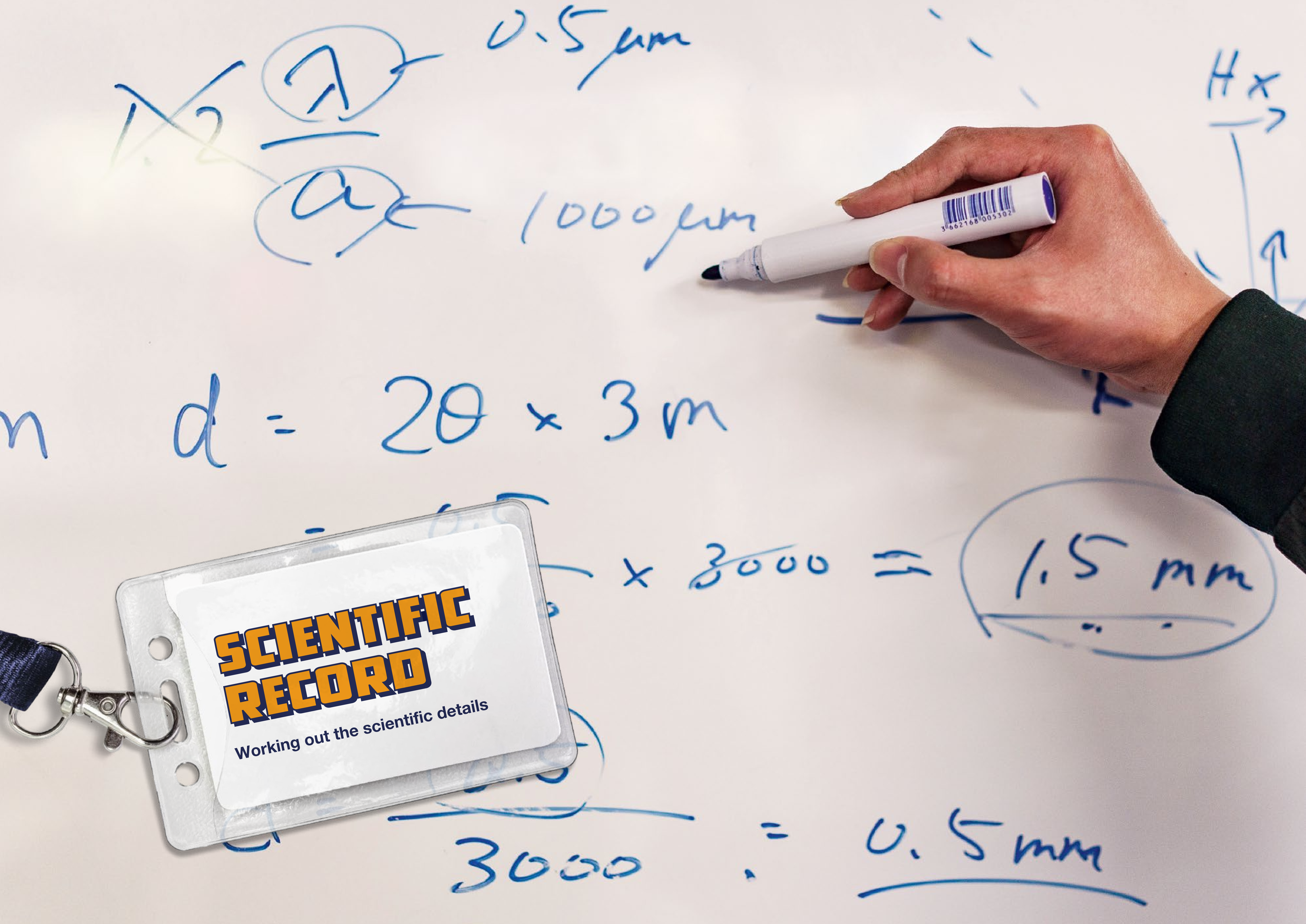

SCIENTIFIC RECORD
Working out the scientific details
0.5 μm
1000 μm
d = 20 x 3m
x 3000 = 1.5 mm
3000 = 0.5 mm

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CONFERENCES, WORKSHOPS, AND SEMINARS

Conferences

21–27 JANUARY 2022
European XFEL Users' Meeting

The European XFEL Users' Meeting is an annual opportunity for networking and collaboration between European XFEL and the scientific user community. In 2022, for the second time in a row, the meeting was held as a purely virtual event, jointly with the DESY Photon Science Users' Meeting. Over 2000 scientists from 40 countries registered to participate.

The agenda of the meeting included updates on new developments, plans for the future, scientific highlights from all six instruments, and advancements in instrument design. The programme was complemented by workshops and a presentation of scientific posters. Many of the research results presented provided new approaches to solving societal challenges, such as the COVID-19 pandemic, a circular economy, artificial photosynthesis, and sustainable catalysis. A highlight of the event was the announcement of the winner of the European XFEL Young Scientist Award, which was awarded for the second time.

28 MARCH – 1 APRIL 2022
14th International Conference on Synchrotron Radiation Instrumentation 2021

More than 1160 participants met virtually from 28 March to 1 April for the 14th International Conference on Synchrotron Radiation Instrumentation (SRI2021), organized by DESY and European XFEL, which had to be postponed until 2022 because of the COVID-19 pandemic. The triennial conference is a prime forum to highlight connections between synchrotron radiation instrumentation, science, and society. It also provides opportunities for discussion and collaborations among scientists and engineers around the world involved in the development of new concepts, techniques, and instruments related to synchrotron radiation and FEL research.

Figure 1:
European XFEL Managing Director Robert Feidenhans'l speaking at SRI2021

19–22 SEPTEMBER 2022
Science@FELs 2022

The Science@FELs 2022 conference was held at DESY and European XFEL in September with more than 100 participants in attendance from 12 countries. The conference, which is organized every two years by the FELs OF EUROPE collaboration, has evolved into one of the most important international meetings in FEL science. 2022 also marked the 10th anniversary of FELs OF EUROPE.

Figure 2:
Serguei Molodtsov, European XFEL Scientific Director and Chairman of FELs OF EUROPE, held a speech celebrating the 10th anniversary of the collaboration at the Science@FELs 2022 conference.

Workshops

21 JANUARY 2021 – 1 DECEMBER 2022
Virtual Hard X-Ray Collaboration Seminar Series

This series hosted monthly seminars by participating facilities (LCLS, SACLA, European XFEL, DESY, SwissFEL, PAL-XFEL, and, as a guest, SHINE) on a specific topic related to accelerator or photon science. The meetings were spread throughout 2021 and 2022, with lecturers from Germany, the USA, Switzerland, Korea, Japan, and China taking turns presenting topics and chairing the meetings.

1 MARCH 2021 – 6 NOVEMBER 2023
FELs OF EUROPE Tutorials

The Science@FELs 2020 conference, the first online Science@FELs, was accompanied by a small number of focus tutorials led by eminent FEL scientists and specifically addressing younger members of the FEL community. The tutorials introduced hot topics in the field of FEL science with more depth than is usually possible in conference talks. Based on the very positive reception of these tutorials, FELs OF EUROPE started a regular online tutorial series inviting distinguished scholars in the field.

24 JANUARY 2022
SXP Instrument at the European XFEL: Status and Perspectives

The Soft X-Ray Port (SXP) is the third instrument at the SASE3 soft X-ray undulator system of the European XFEL. The core idea of the instrument is to extend the portfolio of techniques available at the baseline instruments SCS and SQS. In this workshop, the status of the project and its new scientific perspectives were discussed.

25 JANUARY 2022
Data Analysis at the European XFEL

The experiments at the European XFEL generate enormous amounts of data. While online analysis, which happens in near real time, provides crucial feedback to steer experiments, more rigorous offline analysis is necessary for new scientific findings. The Data Analysis group provides tools that enable analysis and interpretation of data, both online and offline. The aim of this workshop was to introduce the various tools that the group develops, provide examples of their use, and present the views of users. How artificial intelligence and machine learning can be used for data analysis was also discussed.

3–6 OCTOBER 2022
Big Science Business Forum 2022

BSBF is a business-oriented congress that congregates all the European research infrastructures, focused on technology and with the aim to be the main meeting point between research infrastructures and industry. BSBF 2022 was held in Grenada, Spain, co-organized $ by European XFEL.

Figure 3:
European XFEL representatives at BSBF 2022

5 OCTOBER 2022
LEAPS Hour at BSBF 2022

LEAPS Hour, organized by European XFEL, offered participants of the Big Science Business Forum 2022 a unique opportunity to connect with representatives of the League of European Accelerator-based Photon Sources (LEAPS) and with procurement teams. During the event, participants could ask questions, hear about experiences with big science procurement, and discuss ways to collaborate with big science facilities.

2–4 NOVEMBER 2022
Theory Meets XFELs

The aim of this workshop, which was co-organized by European XFEL and held in part on the Schenefeld campus, was to foster collaborations between theorists and experimentalists interested in research with X-ray FELs. It was dedicated to recent theoretical developments in ultrafast X-ray diffraction and imaging, ultrafast X-ray spectroscopy, high energy density physics, ultrafast angle-resolved photoemission spectroscopy, and ultrafast magnetism and was complemented with examples of experimental applications of X-ray FELs in each of these fields.

1–2 DECEMBER 2022
The 2nd Workshop – Towards a Liquid Jet Standardization at European XFEL

This workshop was meant to promote young scientists and Ph.D. students from the microfluidics research environment, facilitating collaboration and networking. International experts as keynote speakers and invited speakers focused on “High repetition rate vs. sample efficiency” and “Synergies between XFEL and synchrotron on liquid jets”. The workshop was held as a hybrid meeting with onsite and digital participation options. The programme for onsite participants included round-table talks on sample delivery topics.

Seminars

THEORY SEMINARS

20 JANUARY 2022
Theoretical insights into ultrafast thermometer and the approach to equilibrium in pump/probe experiments
Jim Freericks, Georgetown University (USA)

5 MAY 2022
Materials discoveries at extreme conditions: from curiosity-driven research to advanced functionalities
Igor Abrikosov, Linköping University (Sweden)

12 SEPTEMBER 2022
Monitoring elementary molecular events by ultrafast nonlinear X-ray spectroscopy
Shaul Mukamel, University of California, Irvine (USA)

1 NOVEMBER 2022
Predictions of novel features in X-ray scattering spectra for thermometry
Alina Kononov, Sandia National Laboratories (USA)

SCIENCE SEMINARS

11 JANUARY 2022
Dynamics and chemical reactivity at aqueous interfaces
Damien Laage, Ecole Normale Supérieure (France)

18 JANUARY 2022
Ultrafast magnetism – terra incognita beyond the classical approximations
Aleksei V. Kimel, Radboud University (The Netherlands)

8 FEBRUARY 2022
Sustainable hydrogen technologies for future energy systems
Robert Schlögl, Max Planck Institute for Chemical Energy Conversion (Germany)

22 FEBRUARY 2022
Facilities: How to avoid running out of samples by rethinking their role
James H. Naismith, University of Oxford (UK)

22 MARCH 2022
Catalysis for a clean and sustainable future: Dynamics on different time and complexity scales
Jan-Dierk Grunwaldt, Karlsruhe Institute of Technology (Germany)

19 APRIL 2022
Watching and directing electrons on the atomic level to understand quantum dynamics from attoseconds to femtoseconds, and beyond
Thomas Pfeifer, Max Planck Institute for Nuclear Physics (Germany)

3 MAY 2022
Ultrafast-electron-diffraction studies of materials at extreme conditions: from ultrafast melting to radiation damage and plastic deformation
Siegfried Glenzer, SLAC National Accelerator Laboratory (USA)

17 MAY 2022
Fast electrons and hard X-rays for unraveling charge carrier dynamics
Renske van der Veen, Helmholtz-Zentrum Berlin (Germany)

31 MAY 2022
Ultrafast nonadiabatic dynamics of nucleobases
Gühr Markus, University of Postdam (Germany)

14 JUNE 2022
New preparation methods based on superhydrophobic phenomena compatible with XFEL investigation methods
Enzo Di Fabrizio, Politecnico di Torino (Italy)

5 JULY 2022
Ultrafast multiplex electron cinema with soft X-ray laser flashes at SASE3/SXP
Kai Rossnagel, Kiel University and DESY (Germany)

5 SEPTEMBER 2022
Superconductivity: One hundred years to reach room temperature
Warren E. Picketty, University of California, Davis (USA)

13 SEPTEMBER 2022
Tracing ultrafast electron dynamics in isolated nanoparticles with coherent diffraction imaging
Daniela Rupp, ETH Zurich (Switzerland)

29 NOVEMBER 2022
Tracking a phase transition from atomic to nanoscopic length scales
Simon Wall, Aarhus University (Denmark)

13 DECEMBER 2022
Q&A with editors of Nature and Nature Physics
David Abergel *(Nature Physics)*, Stefanie Reichert *(Nature Physics)*, and Tobias Rödel *(Nature)*

GLOSSARY

A

AGIPD
Adaptive Gain Integrating Pixel Detector
[European XFEL detector]

B

BMBF
Federal Ministry of Education and Research in Berlin, Germany

C

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

CERN
European Organization 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

DAFHES
Danish Agency for Higher Education and Science in Copenhagen, Denmark

DESY
Deutsches Elektronen-Synchrotron in Hamburg and Zeuthen, Germany

DFG
German Research Foundation

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

FTE
full-time equivalent

FXE
Femtosecond X-Ray Experiments
[European XFEL instrument]

H

HED
High Energy Density Science
[European XFEL instrument]

HiBEF
Helmholtz International Beamline for Extreme Fields at the European XFEL

HZDR
Helmholtz-Zentrum Dresden-Rossendorf, Germany

I

INFN
Istituto Nazionale di Fisica Nucleare in Rome, Italy

L

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

LPD
Large Pixel Detector
[European XFEL detector]

M

MID
Materials Imaging and Dynamics
[European XFEL instrument]

N

NCBJ
National Centre for Nuclear Research in Świerk, Poland

NRC KI
National Research Centre "Kurchatov Institute" in Moscow, Russia

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

P

PETRA III
Synchrotron radiation facility at DESY in Hamburg, Germany

PSI
Paul Scherrer Institute in Villigen, Switzerland

R

RMS
root mean square

S

SASE
self-amplified spontaneous emission

SASE1, SASE2, SASE3
FEL undulator beamlines at the European XFEL

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]

SXP
Soft X-Ray Port
[European XFEL instrument]

U

UKRI
UK Research and Innovation in Swindon, UK

V

VR
Swedish Research Council in Stockholm, Sweden

EUROPEAN XFEL ANNUAL REPORT 2022

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European X-Ray Free-Electron Laser Facility GmbH, May 2023

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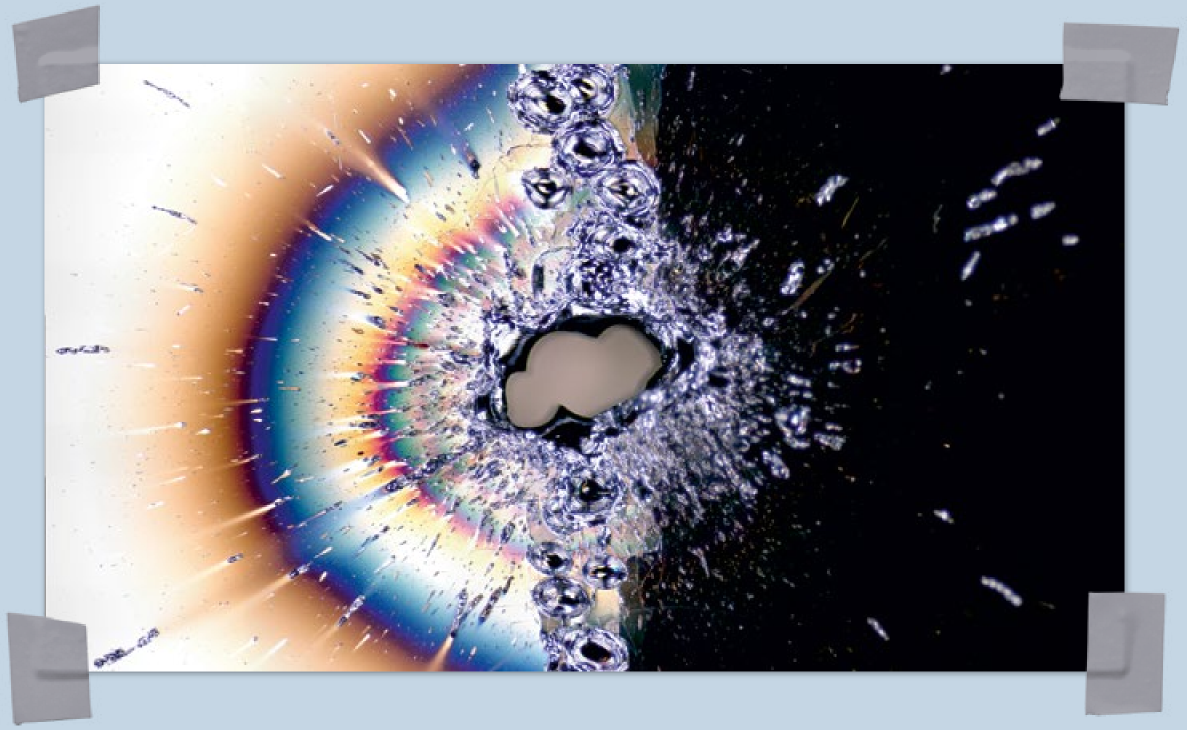

Figure 1:

This photo, showing a microscopic image of a SASE1 absorber crystal, was taken at the FXE instrument by Carsten Deiter with the active support of Martin Knoll. The image shows a silicon attenuator situated in one of the European XFEL beamlines to reduce the power of the incoming X-ray radiation. In the case of this crystal, the power of the beam has caused the silicon to become damaged, leaving a cracked surface, molten remains and an iridescent oil-spill type pattern. The image was named overall winner of the 2022 European XFEL photo festival, an award judged by both staff and a panel of judges.

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