European XFEL

ANNUAL REPORT 2021

Developments, Results, Impressions

European XFEL Annual Report 2021

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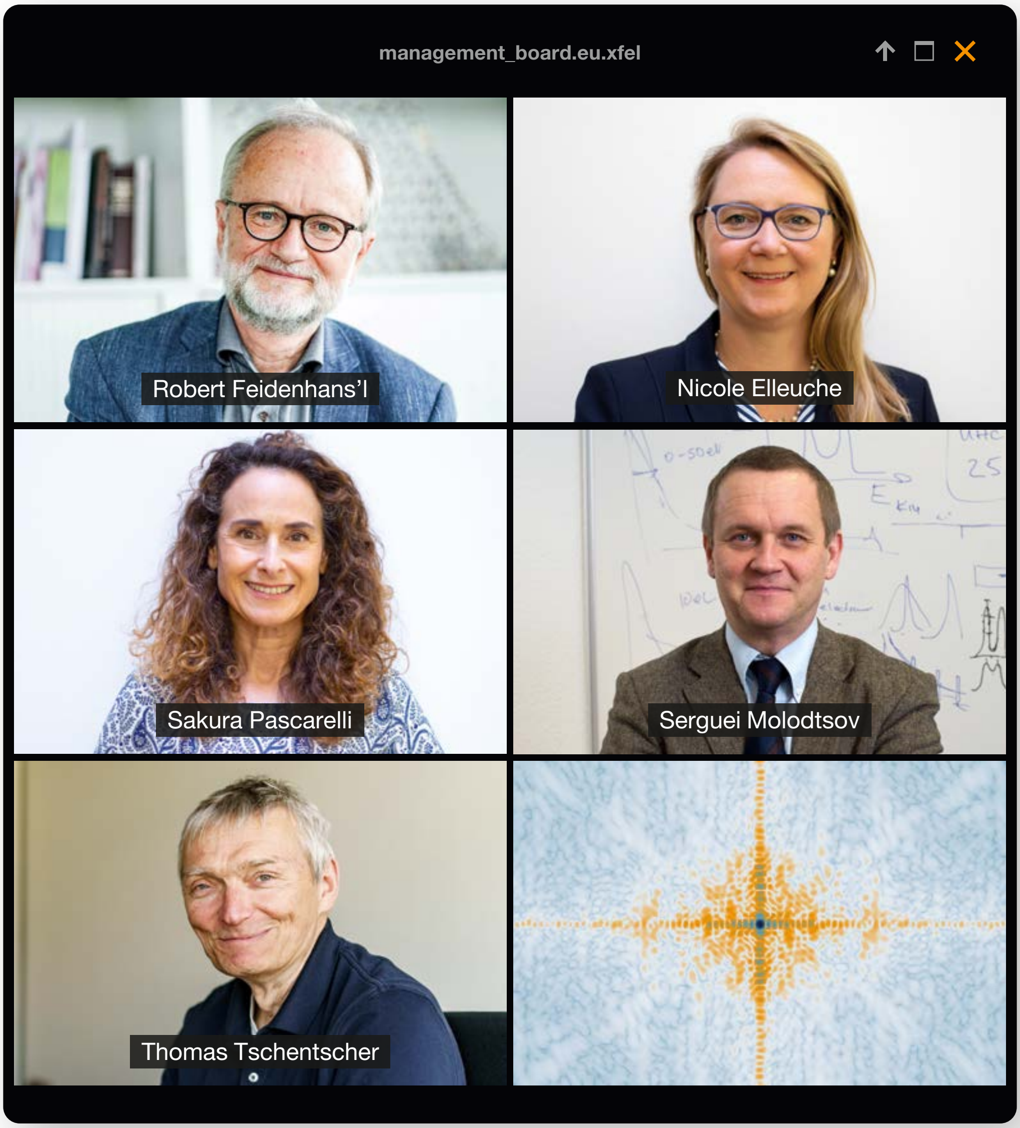
Management Board Foreword



It is with a certain amount of pride that we write this foreword for the Annual Report 2021. Given that the COVID-19 pandemic determined the boundaries of operation in the first half of 2021, this has been a very good year indeed.

The start of regular user operation was delayed slightly, but we caught up quickly, in particular after the summer maintenance period. Many users participated remotely, but many were also on site, staying in the new guest house, and many excellent user experiments were performed. We are getting better and better at conducting experiments with users participating mostly remotely, even though it is much more demanding for our staff.

We look forward to seeing more users on site again in 2022, most likely in the second half of the year. We also eagerly look forward to the data analysis and publications related to the experiments carried out in 2021, some highlights of which you will find in this annual report.

For the first time, the annual report also includes a description of our Ph.D. programme. About 50 Ph.D. student positions, partly or fully financed by us (including third-party funding), are available at European XFEL, and we are setting up a common framework for their studies and research. Training the scientists of tomorrow is one of our core missions.

To help in the fight against the COVID-19 pandemic—which may continue for several years—we launched a special call for proposals in 2020, and three COVID-19–related experiments were conducted with priority at the beginning of 2021. This was the first time we made a thematic call for proposals. It went very well, we learned a lot, and we will continue to use this tool in the coming years to address other strategic topics.

More novelties introduced in 2021 included the Data Operation Centre (DOC), the priority access mode, and the hRIXS instrument. First, the DOC solved problems in real time during operation with experiments, and it has been very successful in quickly resolving various data problems, including those related to detectors and motors. Detector operation was very stable throughout the year without major disturbances. In the last week of the user run, more than 5 PB of raw data was produced without major problems in storage, although there were challenges. The second novelty, the priority access mode—in which one instrument at a given SASE beamline has priority 24 hours a day—was also very effective and prevented the time loss caused by retuning the beam twice a day. Priority access mode will continue in 2022. Finally, with the successful commissioning of the hRIXS instrument, new capabilities for high-resolution inelastic scattering have been added to the experiment programme.

It is a particular pleasure to report on the operation and performance of the linear accelerator. It worked very reliably throughout 2021, with very few disturbances to the user programme. At the same time, the accelerator staff made significant advances in the photon delivery capabilities, such as achieving lasing at 30 keV photon energy, providing stable self-seeding options for the user programme, enabling two-colour operation mode, and easing operational constraints on the pulse delivery in the experiment hall.

The European XFEL strategy process gained a lot of momentum in 2021, even though it was difficult for the teams to meet in person during most of the year. Strategic directions are emerging for the future development of the accelerator, the experiment programme, and the development of staff, and we look forward to presenting more details in next year's annual report. In the current annual report already, you will notice a stronger emphasis on our contributions to the societal challenges we all face. This will be a major focus of the new strategy.

A special highlight in 2021 was that Spain, which was one of our founding shareholder countries, finally became a full member of European XFEL. This achievement was underlined by the increasing number of Spanish users from many different fields. This is very promising for the future Spanish user community, and we look forward to this collaboration in the coming years.

We would like to thank our Council and our committees for their help and strong support during the very difficult circumstances in 2020–2021, when in-person meetings rarely took place and offline discussions over a cup of coffee were absent. Videoconference fatigue resulted, but we are convinced that 2022 will be better—although we are careful not to use the word "much". We hope that many more meetings will take place in person again this year.

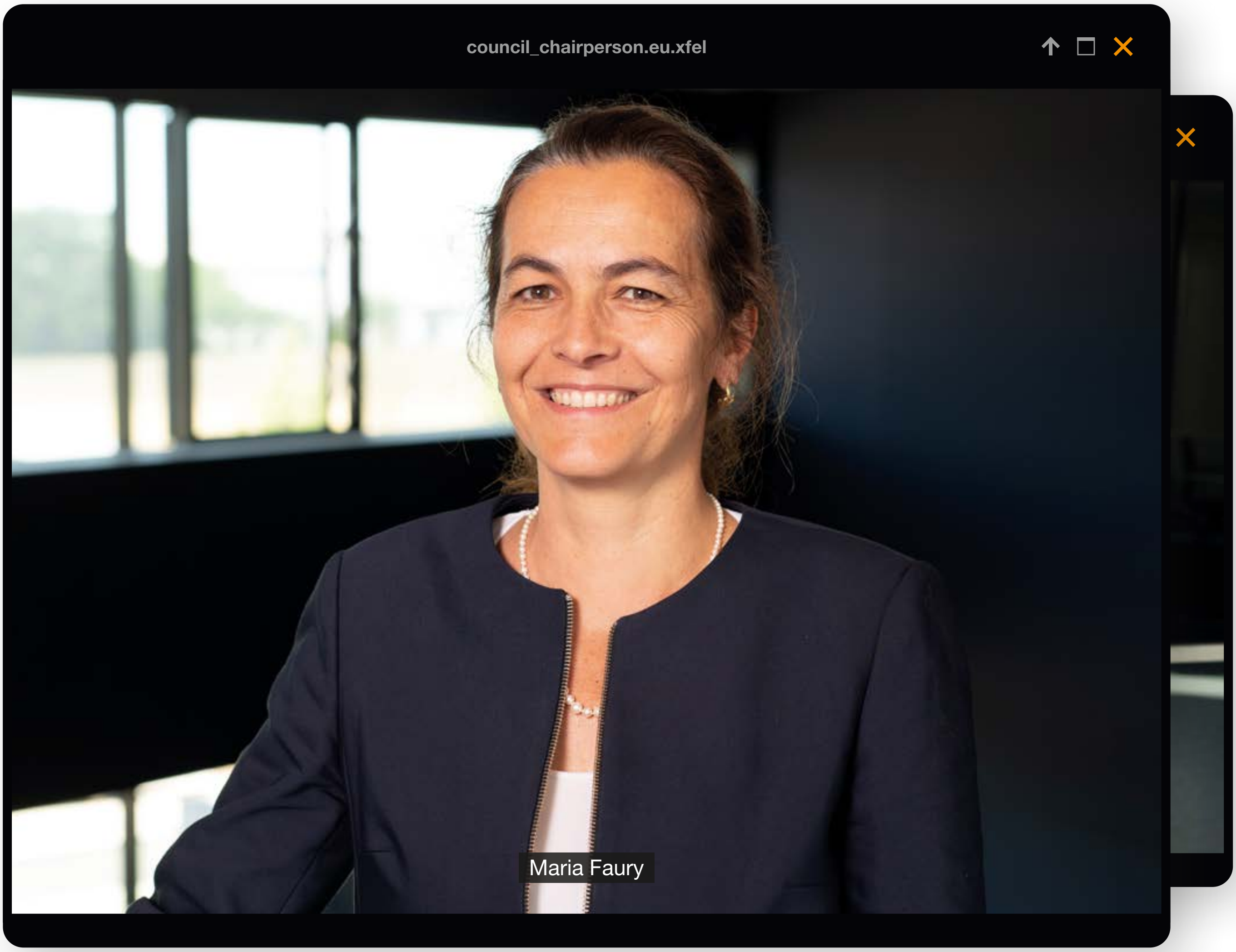
Finally, we would like to thank our users, who continue to conduct exciting experiments at the European XFEL under challenging circumstances, and in particular our staff and our colleagues at DESY for their commitment and energy, which helped turn 2021 into a success despite the difficulties caused by the pandemic.

Robert Feidenhans'l **Nicole Elleuche**

Managing Directors

Serguei Molodtsov **Sakura Pascarelli** **Thomas Tschentscher**

Scientific Directors


council_chairperson.eu.xfel
Maria Faury

Council Chair Foreword

At the time of this writing, while the omicron coronavirus variant is spreading rapidly in Europe, one might feel downcast at the prospect of once again telecommuting, social distancing, and masking. But the virus does not have a monopoly on contagion! Optimism is contagious too. So let's keep our spirits light and our smiles bright. There is light is at the end of the (European XFEL) tunnel!

Looking back at 2021, we have good reason for optimism. First, a robust path for Spain to become full a European XFEL member was found, providing a clear and positive outcome to a longstanding issue.

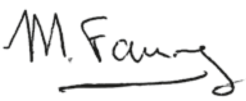
Despite the COVID-19 pandemic and all the burdens it entailed, thanks to restricted access and adapted work instructions, the European XFEL management and staff upheld the performance and progress of the facility. A total of 4664 hours of beamtime were delivered to users in 583 shifts; 44 user experiments were carried out with 220 users on site, and many more participating remotely. In the name of the Council, I would like to thank everyone involved for making all of this possible under such difficult circumstances.

In the summer, the guest house opened its doors, welcoming more than 170 guests during the remainder of the year. The European XFEL Council Vice Chairman, Martin Meedom Nielsen, and I had the opportunity to be the first guests during the June Council meeting—and, I must say, it is a really nice place to stay.

In September, Robert Feidenhans'l's contract was renewed in Paris, extending his duties as Chairman of the Management Board until the end of 2023. I wish him all the best for the next two years, as he faces the task of bringing the facility up to its full capacity while preparing the next steps with the European XFEL Strategy 2030+.

Some changes are foreseen in the European XFEL governance. I am happy to announce that Federico Boscherini will take over as the new Chairman of the Council at the completion of my second term, at the end of June 2022. I wish him as much pleasure as I have had in chairing such a stimulating and active council. I would also like to welcome Claudio Masciovecchio and Evgeny Levichev, our new Chairmen of the Scientific Advisory Committee (SAC) and the Machine Advisory Committee (MAC), respectively, and to express my sincere thanks to Ian Robinson and Andy Wolski for their tremendous work and great success in chairing these committees during the past three years.

Again, I would like to thank the management, the staff, and the governance bodies of European XFEL for their deep involvement and strong commitment to the success of the facility. And, if I may quote Bob Marley, thank you all for "lighting up the darkness"!



Maria Faury, 13 January 2022

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NEWS AND EVENTS

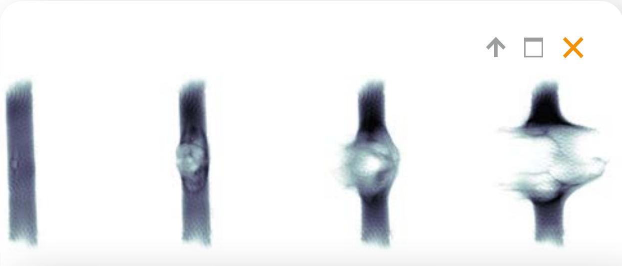
COVID-19–related beamtime at SPB/SFX

News and Events

4 January

Exploding water jet in X-ray beam

A team of scientists, led by Johannes Hagemann from DESY, used the European XFEL's ultrashort X-ray pulses to image rapidly exploding jets of water by means of X-ray holography. The images published in the *Journal of Synchrotron Radiation* revealed the detailed dynamics of the exploding jet. The experiment at the European XFEL's MID instrument demonstrated that water jets are suitable for carrying larger objects, such as intact, live cells, into the X-ray beam. The advantage of using water is that the cells remain in an aqueous environment and do not have to be immobilized or dried.



Water jet 1, 5, 10, and 20 ns after being struck by an infrared laser

4 January

Clear path to better insights into biomolecules

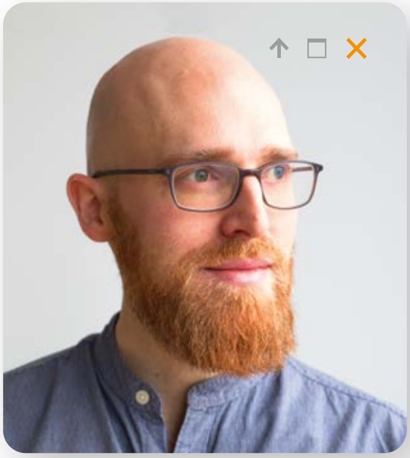
An international team of scientists, led by Kartik Ayyer from the Max Planck Institute for the Structure and Dynamics of Matter, Germany, obtained some of the sharpest possible 3D images of gold nanoparticles. The results of the experiment, which was carried out at the European XFEL's SPB/SFX instrument, were published in the journal *Optica* and lay the foundation for taking high-resolution images of macromolecules such as carbohydrates, lipids, proteins, and nucleic acids, which are vital for life.

Illustration of a 3D diffraction pattern of octahedral nanoparticles obtained by combining many snapshots after structural selection

27 January

First European XFEL Young Scientist Award

Michael Schneider from the Max Born Institute in Berlin received the newly established European XFEL Young Scientist Award. Schneider has worked on several experiments at the European XFEL's SCS instrument since the start of its user operation. He received the award in recognition of his excellent research focused on ultrafast magnetization dynamics.



27 January

Virtual Users' Meeting with 2000 registered participants

The 2021 European XFEL Users' Meeting was different from previous years: it was held virtually. But that did not diminish the numbers; it remained one of the largest meetings of its kind worldwide. A total of around 2000 scientists from 40 countries registered for the DESY Photon Science and European XFEL Users' Meetings, which took place in parallel. The European XFEL meeting focused on the scientific highlights, progress, and current status of the X-ray laser facility. It was complemented by satellite meetings, workshops and a scientific poster presentation.

2 April

X-ray screening for COVID-19 drugs

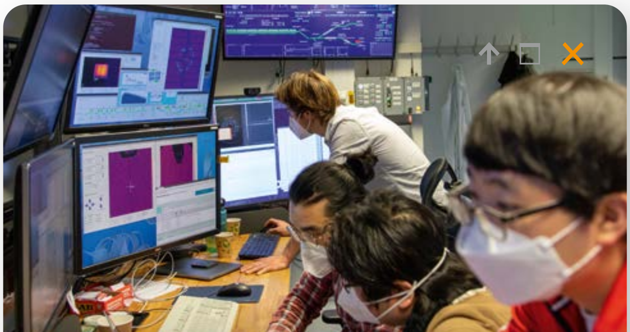
A team of over 100 researchers, including scientists from European XFEL, identified several candidate drugs that could potentially be used against the SARS-CoV-2 coronavirus. They successfully screened 6000 active substances already in use for treating other diseases; the results were published in *Science*. The team, led by DESY physicist Alke Meents, screened substances that bind to an important protein of SARS-CoV-2 and could therefore be the basis for a drug against COVID-19. They identified 37 substances that bind to the main protease of the virus. The scientists at European XFEL supported the screening process remotely and performed follow-up experiments to verify the outcome.

Christina Schmidt, a co-author of the publication and a research assistant in European XFEL's Sample Environment and Characterization group

20 April

Beaming in on coronavirus details

Starting in March 2021, three experiments received COVID-19–related beamtime at the European XFEL's SPB/SFX instrument. Two collaborations, led by scientists from DESY and the Diamond Light Source, looked at the structure and the binding of ligands to the proteases of the SARS-CoV-2 coronavirus. A third collaboration, led by the European Molecular Biology Laboratory (EMBL), studied the viability of small-angle X-ray scattering at the European XFEL, which could be used to examine proteins without the need for crystallization (see 6 July). The experiments were successful, although very few users were able to be on site due to the pandemic situation.

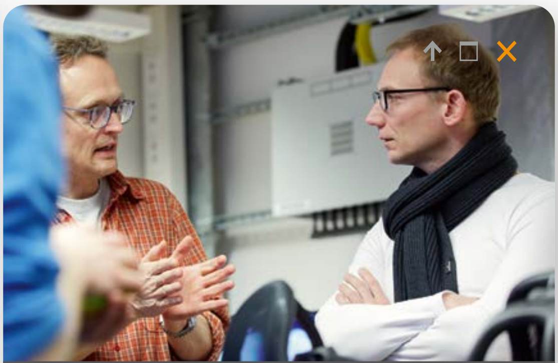


Control hutch during one of the first COVID-19–related beamtimes at the SPB/SFX instrument

6 May

Andrea Eschenlohr chairs the User Organization

Andrea Eschenlohr from the University of Duisburg-Essen, Germany, is the new Chairwoman of the Executive Committee of the European XFEL User Organization. The former Vice Chairwoman took over from Allen Orville of the Diamond Light Source, Oxford, UK, as scheduled after his two-year term ended. Orville had been the Chairman of the Executive Committee since the User Organization was founded in 2019. Robert Grisenti of the GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt, Germany, will be the new Vice Chairman. The European XFEL User Organization is an independent association of scientists with the goal to improve conditions for users and help expand the user community.



Robert Grisenti (r.) at a user run

Andrea Eschenlohr at the Users' Meeting 2020

14 May

Shortcut to high-density materials

An international group of researchers pioneered a new way of performing static high-pressure and high-temperature experiments, using diamond anvil cells at the European XFEL's HED instrument, and discovered a new, faster route to produce iron nitrides—promising candidates for high-density data storage and other applications. The scientists reported their results in the *Journal of Physical Chemistry Letters* and the *Journal of Synchrotron Radiation*. They followed the reaction of iron foil with nitrogen under X-ray bombardment at 50 000 times atmospheric pressure. Systematic exploration of chemical reactivity at extreme pressures and temperatures is expected to lead to the discovery of unknown pathways to industrially relevant compounds and to compounds that are needed to understand the chemistry of astrophysical objects and processes.

Experiment chamber at the European XFEL's HED instrument

8 June

X-ray imaging of bubbles and shockwaves in water

Everyone is familiar with tiny gas bubbles gently rising in sparkling water. The bubbles created by intense focused lasers at the European XFEL's MID instrument, however, were 10 times smaller and contained water vapour at a pressure around 100 000 times higher. Under these conditions, the bubble expands at supersonic speed with a shockwave consisting of a spherical shell of highly compressed water. A research team led by the University of Göttingen, together with DESY and European XFEL, described in *Nature Communications* how they used holographic flash imaging and nanofocused X-ray laser pulses to capture data and images, leading to a "movie" of the process. The technique can provide insights for applications such as laser processing of materials, modification of chemical reactions, or laser surgery.

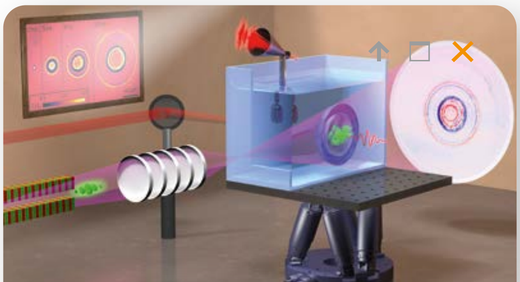


Illustration of the experiment

21 June

European XFEL guest house inaugurated

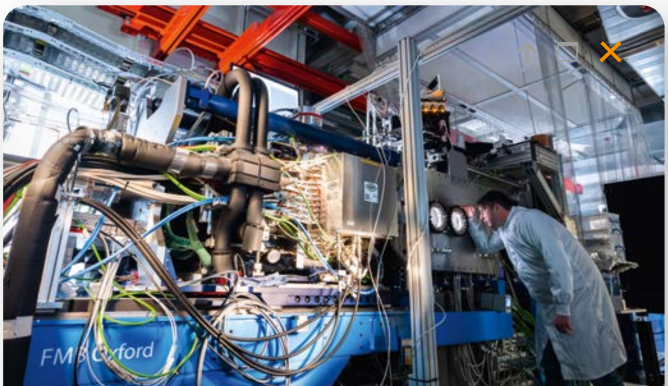
Katharina Fegebank, Science Senator of Hamburg, together with Friederike Kampschulte, Head of the Science Department at the Ministry of Education, Science and Culture of Schleswig-Holstein, opened the European XFEL guest house on the Schenefeld research campus. The new guest house has 58 beds in 55 rooms and can be used outside of beamtimes for other guests of the research facility or eventually for events at the planned visitor centre. The rooms display artistic images of various elements and sections of instruments and components of the X-ray laser.

Left to right: Robert Feidenhans'l, Nicole Elleuche, Friederike Kampschulte, and Katharina Fegebank in front of the guest house

6 July

Insights into coronavirus proteins

A collaboration led by researchers from the European Molecular Biology Laboratory (EMBL) used small-angle X-ray scattering (SAXS) at the European XFEL's SPB/SFX instrument to obtain data on samples containing SARS-CoV-2 spike proteins, including proteins of the isolated receptor binding domain. SAXS is a powerful technique, as it allows researchers to gain insights into protein shape and function at microscales and nanoscales. It has proven to be extremely useful in investigating macromolecular structures, such as proteins, especially because it removes the need to crystallize these samples. The results can, for example, help scientists to find out how antibodies bind to the SARS-CoV-2 virus and to develop medical strategies to overcome COVID-19.



The SPB/SFX instrument, where the SAXS experiment was carried out

12 July

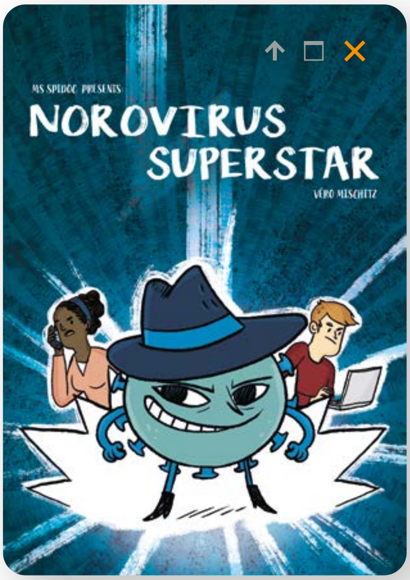
Serguei Molodtsov takes over as FoE Chairman

European XFEL Scientific Director Serguei Molodtsov was appointed Chairman of FELs OF EUROPE (FoE), a collaboration of all free-electron laser (FEL) and short-pulse facilities in Europe, with 15 partner facilities in 11 countries. FoE organizes scientific conferences, such as Science@FELs and PhotonDiag, which bring together users from all partner organizations and facilities.

29 July

Comic book illustrates virus photo shoot

A new comic provides a fun and accessible way to learn more about scientific topics, such as native mass spectrometry and X-ray lasers. "Norovirus Superstar" introduces readers to a range of interesting characters, starting with the anti-hero, the Norovirus. The story helps readers understand what goes on at the European XFEL when snapshots of biological samples are taken. The comic was realized within the MS SPIDOC project, which received funding from the European Union's Horizon 2020 programme.



31 August

HiBEF inaugurated at the European XFEL

Christian Luft, State Secretary at the German Federal Ministry of Education and Research (BMBF), Karin Prien, Minister for Science of Schleswig-Holstein, and Eva Gümbel, State Secretary for Science of Hamburg, inaugurated the Helmholtz International Beamline for Extreme Fields (HiBEF) at the European XFEL.

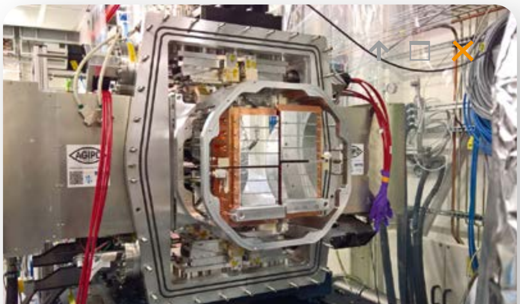
Led by the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) in cooperation with DESY, HiBEF pools equipment and expertise from various research institutions, making them available to the international scientific community. The beamline is part of the HED instrument, enabling deep insights into the structure of materials and hyperfast natural plasma-physical processes. The total investment including operating costs for 10 years amounts to nearly 120 million euros.

The HiBEF interaction chamber is being pushed into the beam.

9 September

Filming antibiotic resistance in slow motion

At the European XFEL's SPB/SFX instrument, an international team of researchers has filmed a reaction step that is important for the development of antibiotic resistance. The molecular movie captures the very rapid reaction of the enzyme beta-lactamase from tuberculosis bacteria with the cephalosporin antibiotic ceftriaxone in slow motion. The team, led by Marius Schmidt of the University of Wisconsin – Milwaukee, USA, published the results in *IUCrJ*, the journal of the International Union of Crystallography. Beta-lactamase can render the most commonly used beta-lactam antibiotics ineffective.



The AGIPD detector at the European XFEL used for the experiment

22 September

Italian ambassador visits European XFEL

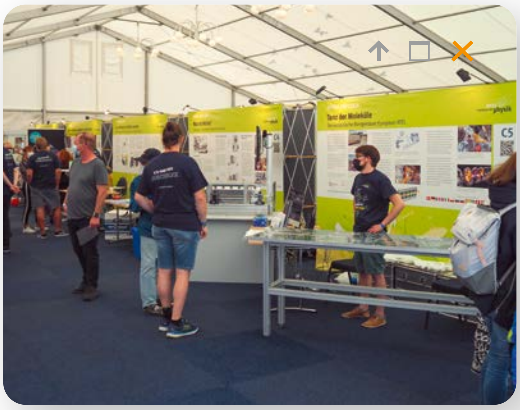
The Italian Ambassador Armando Varricchio and Consul General David Michelut visited European XFEL, meeting Managing and Administrative Director Nicole Elleuche, Scientific Director Sakura Pascarelli, and European XFEL staff members. “Scientific research and experiments at the European XFEL as well as at DESY have a profound impact on scientific progress,” the ambassador said during his visit. “The way information has been shared during the pandemic among scientific communities and the way scientists cooperated worldwide for the research in terms of treatment and vaccination was pivotal for the management of the crisis and, in many cases, represents a blueprint for international cooperation.”

Ambassador Armando Varricchio signing the European XFEL guest book

30 September

European XFEL at “Highlights der Physik”

European XFEL participated in the “Highlights der Physik” science festival in Würzburg from 27 September to 2 October. At the European XFEL stand on the market square, visitors were able to discuss science with staff members and gain insight into current research at the facility. The festival takes place in a different German city every year. In 2021, one focus was X-ray science, and almost all events were broadcast in a live stream and afterwards on demand (in German), including a lecture by European XFEL Scientific Director Thomas Tschentscher. “Highlights der Physik” is organized by the German Federal Ministry of Education and Research, the German Physical Society, and, in 2021, by the University of Würzburg.



18 October

Matteo Porro wins IEEE Award

European XFEL detector development project leader Matteo Porro received the prestigious 2021 IEEE Emilio Gatti Radiation Instrumentation Technical Achievement Award. With the award, the committee honoured Porro’s contributions to the development of soft X-ray imaging detectors suitable for use at X-ray FELs such as the European XFEL. The Institute of Electrical and Electronics Engineers (IEEE) presented the award to Porro at the IEEE Nuclear Science Symposium, held virtually in October.

27 October

US and European science labs collaborate on climate change

Key leaders and researchers from major US and European big science laboratories—EIROforum (Europe’s eight largest intergovernmental scientific research organizations, including CERN, EMBL, ESA, ESO, ESRF, EUROfusion, European XFEL, and ILL) and the US Department of Energy’s 17 National Laboratories (Ames, Argonne, Brookhaven, Fermi, Idaho, Jefferson, Los Alamos, Lawrence Berkeley, Lawrence Livermore, NETL, NREL, Oak Ridge, Pacific Northwest, PPPL, SLAC, Sandia, and Savannah River)—met by videoconference ahead of the United Nations Framework Convention on Climate Change Conference of Parties (COP26) and affirmed their commitment to unite science towards a sustainable and resilient global society and economy.

18 November

LGBTQ+ STEM Day 2021

On the annual International Day of LGBTQ+ People in Science, Technology, Engineering, and Maths (LGBTQ+ STEM Day), European XFEL raised the rainbow flag, shared rainbow cake in the campus restaurant, and encouraged all staff to take part in virtual LGBTQ+ STEM Day events.

24 November

Collaboration agreement with IMDEA Nanociencia signed

European XFEL signed a collaboration agreement with the Madrid Institute for Advanced Studies in Nanoscience (IMDEA Nanociencia), an international multidisciplinary research centre focused on advanced science at the nanoscale established and financed by the Madrid Regional Government. The aim of the collaboration is to strengthen scientific ties between both institutions and help promote X-ray FEL science in Spain. The agreement is also an important milestone towards increasing the participation of Spanish users at European XFEL. IMDEA Nanociencia is one of the founders of the Spain XFEL Hub and employs more than 200 researchers.

Robert Feidenhans'l and IMDEA Nanociencia Director Rodolfo Miranda after signing the agreement in Madrid

25 November

European XFEL campus lights up in orange

On the International Day for the Elimination of Violence against Women, the European XFEL main building and the campus restaurant "BeamStop" were illuminated in bright orange. Together with other landmarks and companies in Schleswig-Holstein, European XFEL participated in the international campaign "ZONTA says NO". The orange light sets a visible sign against violence against women and follows the "Orange the World" campaign of UN Women.

6 December

X-ray laser reveals how radiation damage arises

An international research team used the European XFEL's SQS instrument to gain new insight into how radiation damage occurs in biological tissue. The study revealed in detail how water molecules are broken apart by high-energy radiation, creating potentially hazardous electrically charged ions, which can go on to trigger harmful reactions in the organism. The team, led by Maria Novella Piancastelli and Renaud Guillemin from Sorbonne University in Paris, Ludger Inhester from DESY, and Till Jahnke from European XFEL, presented its observations and analyses in the journal *Physical Review X*.

After the absorption of an X-ray photon, the water molecule can bend up so far that, after only about 10 fs, both hydrogen atoms (grey) are facing each other, with the oxygen atom (red) in the middle.

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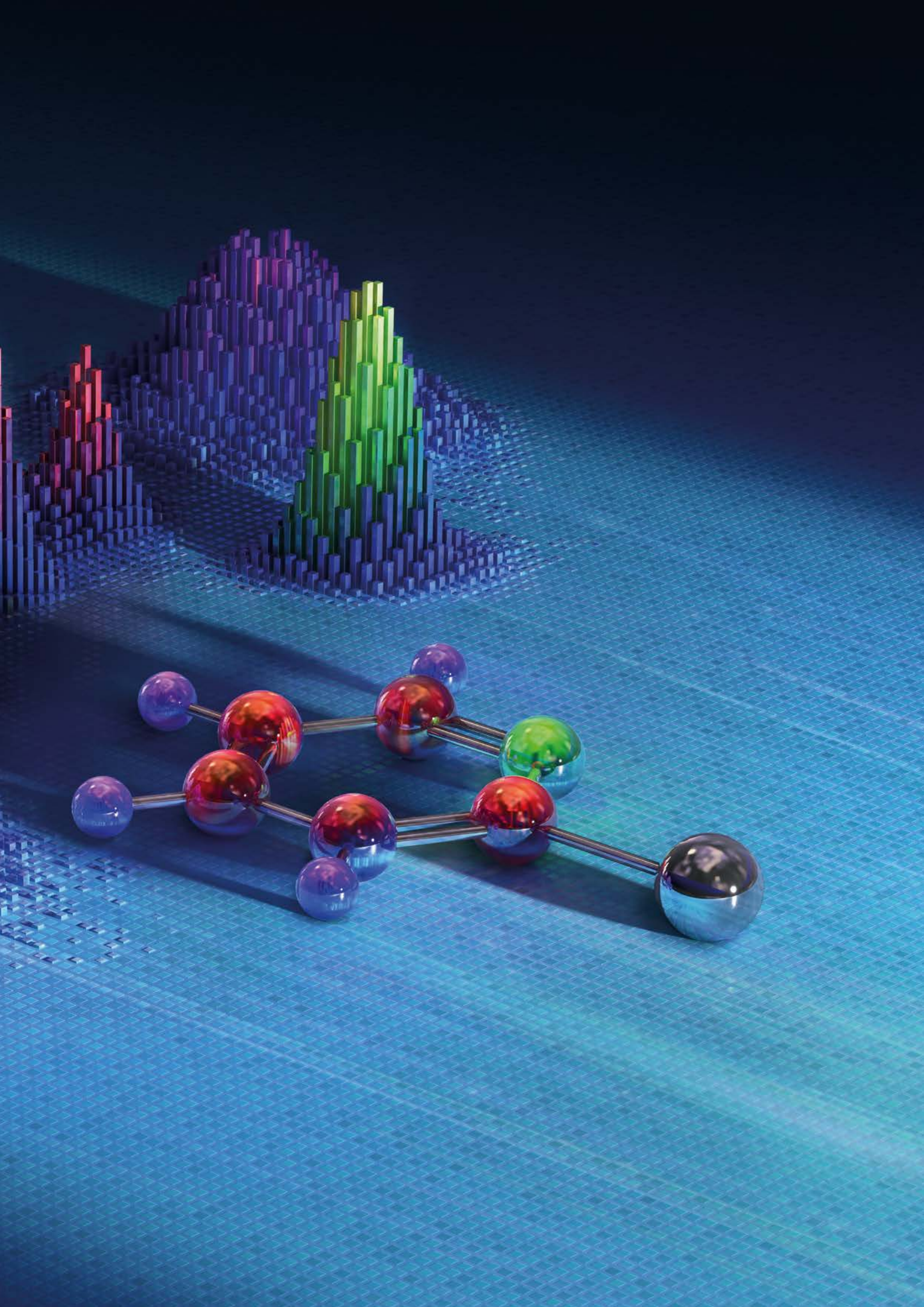
HIGHLIGHTS

Imaging by destruction—visualization of a Coulomb explosion



Studying the elixir of life

Experiments exploring the behaviour of water at high pressure and temperature give new insights into planetary interiors.

Water is essential for life on Earth, and the presence of water on other planets is considered to be an indicator of habitable conditions there too. But while water as a liquid, solid (ice), and gas (steam) is familiar to us all, it also exists in more unusual forms deep in the interior of the Earth and planets further afield. Two recent experiments at the HED instrument explored how and under what conditions water transitions from one form to another, shedding new light onto the interiors of our own and far-flung worlds.

It is thought that deep underground, where extreme pressures and temperatures are found, as much as three times more water could exist than on the Earth's surface. When subjected to the extreme pressure and temperature conditions in the Earth's interior, water takes on unusual forms: bound in minerals, in solid phases not found on the Earth's surface, or as a so-called supercritical fluid. Elsewhere in the universe, both supercritical water and exotic forms of ice are found in the interior of ice giants as well as in planets beyond our solar system.

In order to learn more about the interior dynamics of planet Earth, including how water is transported to the surface via volcanic eruptions and earthquakes, it is essential to understand the behaviour of water at these extreme pressures and temperatures. Modelling the dynamics of icy planets also requires a good knowledge of the behaviour and stability of water under different conditions—in particular, when it is mixed with other compounds, such as ammonia and methane, which are also thought to be present in these planets.

At the HED instrument of the European XFEL, two experiments were recently carried out with the aim of providing new insights into the behaviour of water in different pressure–temperature regimes. "We want to understand what happens at the atomic level when water transitions from one state to another," explains Ulf Zastrau, HED instrument group leader. "Understanding these phase transitions is a first step towards determining the physical properties of water at a given depth within a planet."

"The pressure and temperature over which water phases are stable provide information about the form that water adopts at a given depth within the planet," explains DESY scientist Hanns-Peter Liermann, principal investigator of one of the two experiments carried out at HED. This is particularly important in the case of a type of ice known as superionic ice, in which protons can move freely within the oxygen lattice, which has important implications for a planet's magnetic field.

fig-1_miniature-heaters.png

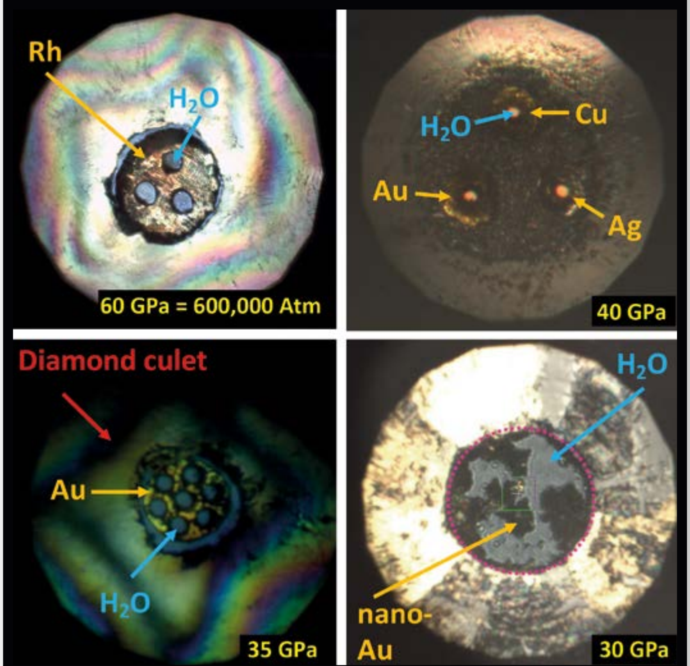


Figure 1:
Miniature heaters constructed from different materials and in different geometries on the tip of a diamond anvil (diameter 300 µm). The heaters were used to dynamically heat samples of water by means of the European XFEL pulses. The figure shows samples prepared for the DAC community user experiment #2590 by the University of Edinburgh (UK), DESY (Germany), the Carnegie Science Earth and Planets Laboratory (USA), the University of Chicago (USA), and Argonne National Laboratory (USA).

fig-2_HED-experiment-setup.ppt

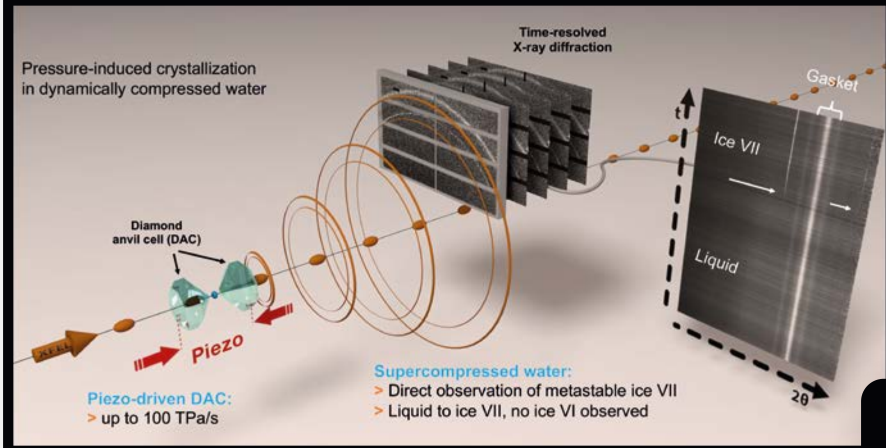


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Figure 2:
Setup of the second experiment at HED, illustrating how time-resolved X-ray diffraction measurements allowed the observation of pressure-induced crystallization of water as it was dynamically compressed using a piezo-driven dynamic DAC

However, recreating these extreme pressures and temperatures is far from trivial. “The study of water at such extreme pressures is possible in the laboratory using diamond anvil cells, or DACs, which can compress materials to pressures of more than 100 GPa, or approximately one million times atmospheric pressure,” explains Malcolm McMahon from the University of Edinburgh, UK. The intense X-ray pulses from the European XFEL are then used to measure the structure of the sample.
The experiments at HED used two different approaches: dynamic heating and dynamic compression.

In a first experiment exploring dynamic heating, the scientists used the unique rapid succession of X-ray flashes generated by the European XFEL to perform step-wise X-ray heating, where each pulse probes the heated state created by the previous pulse—an experiment setup not possible before the advent of X-ray FELs (Figure 1). “High-temperature experiments at synchrotrons are complicated by the fact that water is chemically reactive,” explains McMahon, who led the dynamic-heating experiment. “Water generally doesn’t scatter X-rays very well, so very long exposure times were required to keep the sample hot enough for the measurements, leading to unwanted chemical reactions. For this experiment at HED, we were able to use the intense, ultrashort-time-scale X-ray pulses produced by the European XFEL to successfully obtain high-quality diffraction patterns from the samples from a single X-ray laser pulse.” Rachel Husband, scientist from DESY and one of the leading scientists of the study, adds: “This mitigated some of the challenges encountered in previous experiments, demonstrating that we can create highly reactive, high-temperature states, such as superionic ice, while simultaneously allowing us to probe the structure of these exotic phases.” In the future, the successful setup will be extended to study mixtures with ammonia and methane, which are more relevant for planetary science.

In the second experiment, the team performed time-resolved studies of dynamically compressed water (Figure 2). High-pressure behaviour has been studied before, but the setup at HED enabled the scientists to probe the structural behaviour of the samples while these were being compressed in the DAC. “This experiment successfully demonstrated that the European XFEL can be used to study samples as they are dynamically compressed using DACs, where the compression time scale is comparable to the length of the pulse train,” says Liermann. This opens up the possibility for future studies exploring crystallization, kinetics, and metastability in low-scattering materials, such as water and its mixtures.

Authors

The work on dynamic heating is presented on behalf of the community user experiment #2590 (principal investigator: M.I. McMahon; main proposer: R.J. Husband). The work on dynamic compression is presented on behalf of the community user experiment #2592 (principal investigator: H.P. Liermann; main proposer: Z. Jenei). Both experiments were performed at the HED instrument of the European XFEL.

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Antibiotic resistance captured on film

Molecular movies reveal how bacteria evade antibiotics, offering clues on how to design new drugs—for example against antibiotic-resistant tuberculosis.

For the past century, antibiotics have revolutionized healthcare across the globe. However, as more (multi-)antibiotic-resistant strains of bacteria emerge and become prevalent, a "post-antibiotic" era is a real and dire possibility. Structural-biology techniques, such as crystallography, enable scientists to map the 3D atomic structure of bacterial molecules, such as proteins, in order to glean crucial information about how they cause disease and, in turn, how to design new drugs to disarm them. The extremely bright, high-repetition-rate X-ray flashes generated by the European XFEL now open up the possibility to go beyond static images of molecules, generating "molecular movies" that reveal details of how molecules interact with each other throughout the infection process and how drug molecules can alter and stop that process. In an experiment at the SPB/SFX instrument, an international team of scientists used a novel sample injection method in combination with the unique X-ray pulses of the European XFEL to study the reaction of an enzyme known as beta-lactamase from the bacterium *Mycobacterium tuberculosis* together with the cephalosporin antibiotic ceftriaxone. Their work demonstrated the potential of this technique for biomedical research.

A recent analysis of the global burden of antimicrobial resistance (AMR) revealed that more than 4.9 million people died in 2019 as a direct or indirect result of AMR [1]. This most comprehensive study of its kind shows that AMR, including antibiotic resistance, has become the leading cause of death worldwide. Tuberculosis, caused by the bacterium *Mycobacterium tuberculosis* (Mtb), is a preventable and curable disease, and yet, according to the World Health Organization (WHO), 1.5 million people died of tuberculosis in 2020, making it the second largest cause of death from an infectious disease after COVID-19 [2]. Ending the tuberculosis epidemic by 2030 is one of the United Nations' Sustainable Development Goals. However, multi-antibiotic-resistant strains of Mtb make this a real challenge.

Alongside coordinated action to monitor the use of existing antibiotics, there is an urgent need for research into infection mechanisms to aid the development of new antibiotics. Scientists now have access to a range of structural-biology methods, including crystallography. This uses bright X-ray light to reveal the precise atomic structure of single molecules or groups of molecules, such as bacterial proteins and enzymes together with drug molecules, helping discern their function and identify targets for where drug molecules can attack.

However, beyond static snapshots of molecules, being able to track and observe the entire dynamic process of how a molecule docks onto, enters, alters, and disarms another has long been a dream for structural biologists. The rapid repetition rate of the X-ray pulses generated by the European XFEL now makes molecular movies a real possibility. "By capturing snapshots of sequential phases of the reaction and pasting these images together to create a movie, we can gain valuable insights into how molecules interact," says Adrian Mancuso, group leader of the SPB/SFX instrument at the European XFEL. "Molecular movies have the potential to revolutionize these elements of biomedical research," he adds.

fig-1_SPB-SFX-experiment-setup.png

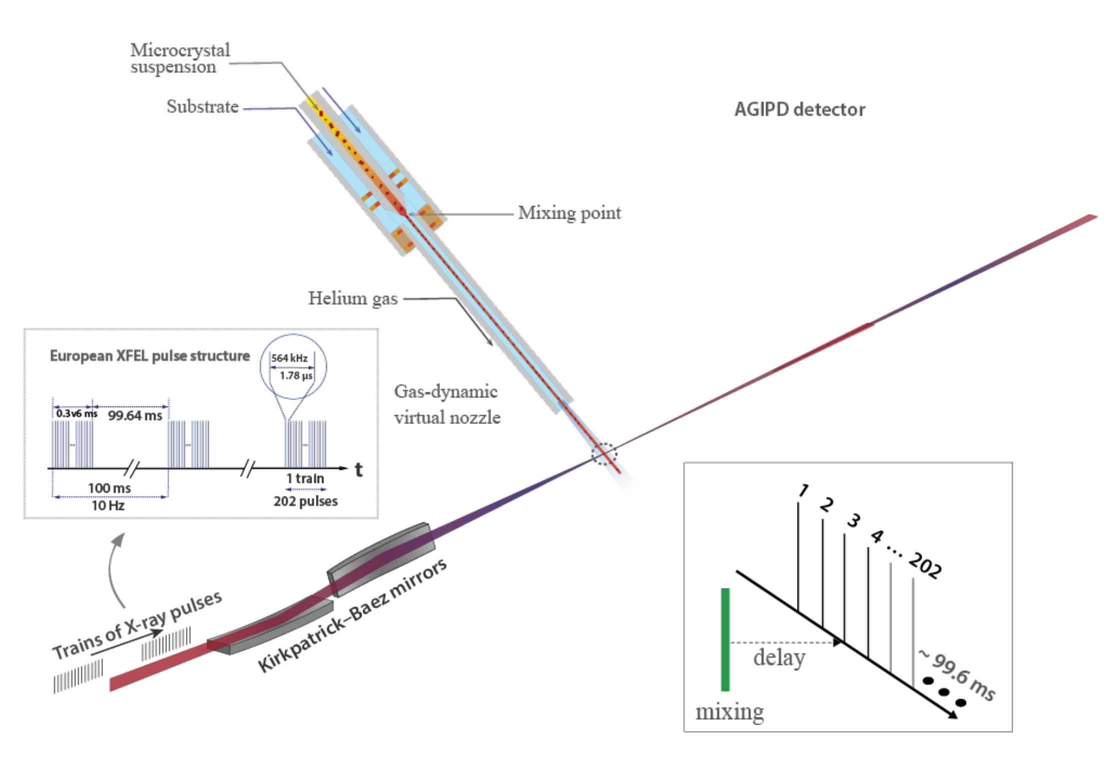

Figure 1:
Experiment setup at the SPB/SFX instrument. Microcrystals of the bacterial enzyme and the drug molecule are mixed with a substrate and injected into the X-ray interaction region (dotted circle) after a specific delay. The mixture is then probed by trains of X-ray pulses from the European XFEL. An AGIPD detector collects the resulting diffraction patterns and reads them out for further analysis.

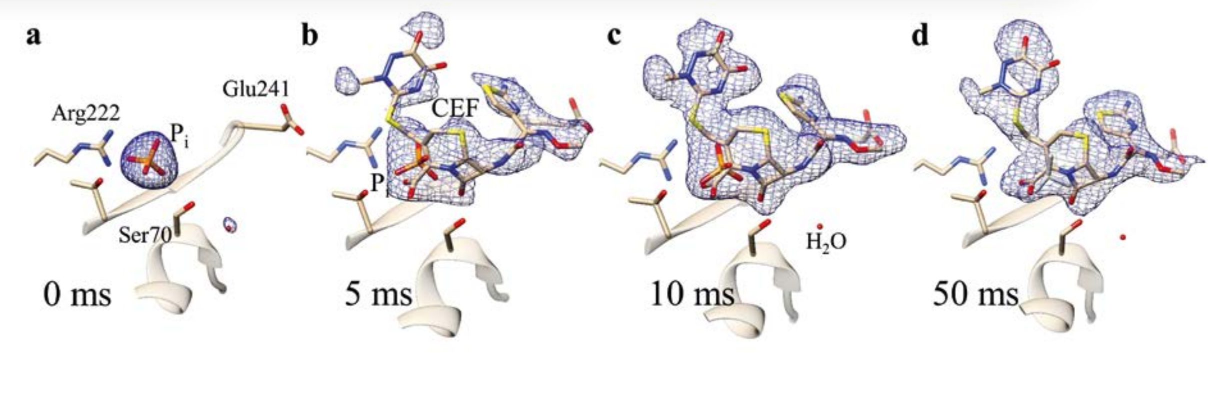

Figure 2:
Initial binding of the antibiotic ceftriaxone (CEF) to the *Mycobacterium tuberculosis* beta-lactamase, determined from the difference electron density in the active centre of the beta-lactamase subunit *B*. (a) The CEF ligand has not yet diffused in; the phosphate (P_i) from the crystallization buffer is dominant in the active site. (b) 5 ms after mixing: The phosphate is beginning to be displaced by CEF. (c) 10 ms after mixing: The phosphate is no longer dominant. (d) 50 ms after mixing: Little evidence of the phosphate remains, and the density only has features of the antibiotic compound. Nearby amino acids are marked in (a).

A team of scientists led by Marius Schmidt from the University of Wisconsin – Milwaukee, USA, made use of the unique parameters of the European XFEL X-ray beam to study how the cephalosporin antibiotic ceftriaxone binds to an enzyme known as beta-lactamase from an antibiotic-resistant strain of Mtb. The enzyme beta-lactamase is found in many strains of bacteria, rendering members of an important class of antibiotics, known as beta-lactam antibiotics, ineffective. “Beta-lactam antibiotics include some of the most commonly and widely used antibiotics, such as penicillin and cephalosporin-based medication, and resistance to these antibiotics poses a real problem,” says Schmidt.

For this study, the scientists trialled a new sample injection method, which involves mixing microcrystals comprising the bacterial enzyme and the drug molecule as they are en route towards the European X-ray beam. By carefully synching the flow rate of the microcrystals with the time frame of the reaction and the pulse rate of the bright X-ray beam, the scientists were able to capture successive snapshots of the reaction in real time (Figure 1), which could then be put together in a molecular movie. Their data revealed new insights into the dynamics within the active site of the enzyme (Figure 2) [3]. The researchers also investigated how an enzyme inhibitor known as sulbactam reacts with the bacterial enzyme. In the case of antibiotic resistance, sulbactam is often administered together with antibiotics, where it binds to the bacterial beta-lactamase, blocking it and thereby restoring the effectiveness of the antibiotics.

“The unique combination of the high repetition rate of the bright X-ray pulses generated by the European XFEL with our novel mix-and-inject technology allowed us to follow the reaction of the *Mycobacterium tuberculosis* beta-lactamase with ceftriaxone in real time,” explains Schmidt. “Our experiment, together with previous results, has shown how X-ray lasers can be used as an important tool for biological research in the future.” The scientists are now keen to optimize the method, using the X-ray pulse train of the European XFEL to collect more data sets.

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Tracking phase transitions in magnetic materials

Tracking the origin of phase transitions in magnetic materials using femtosecond X-ray diffraction could spur the development of effective novel cooling devices, for example for data centres.

Magnetic materials are a key component in many of the devices we use in our everyday lives and, in the quest for greener and more efficient products, they are likely to become even more important. However, there is still much to discover about how they work. Being able to study the structural changes and dynamics that occur within these materials is crucial for their development for applications, such as next-generation data storage devices, efficient refrigeration, and quantum computing. However, for these complex materials, a detailed description of atomic-level processes, such as magnetostructural phase transitions, often remains elusive. The intense X-ray flashes generated by the European XFEL offer new ways to explore such processes. At the FXE instrument, scientists used femtosecond X-ray diffraction to directly track the ultrafast dynamics of structural modifications in manganese arsenide, a material with some fascinating properties.

Manganese arsenide (MnAs) is a very interesting material, characterized for instance by a giant magnetocaloric effect [1], which makes it an attractive candidate in the development of more efficient cooling devices for the household appliance market. It also features colossal magnetoresistance (large resistivity variations induced by applying a magnetic field), a property of interest for spintronic applications [2]. Furthermore, when MnAs is grown in the form of thin epitaxial films on gallium arsenide, it forms a distinctive pattern alternating ferromagnetic and non-ferromagnetic stripes, with potential applications in magneto-acoustics [3] and in magnetization control by light pulses [4].

fig-1_MnA_structure.bmp

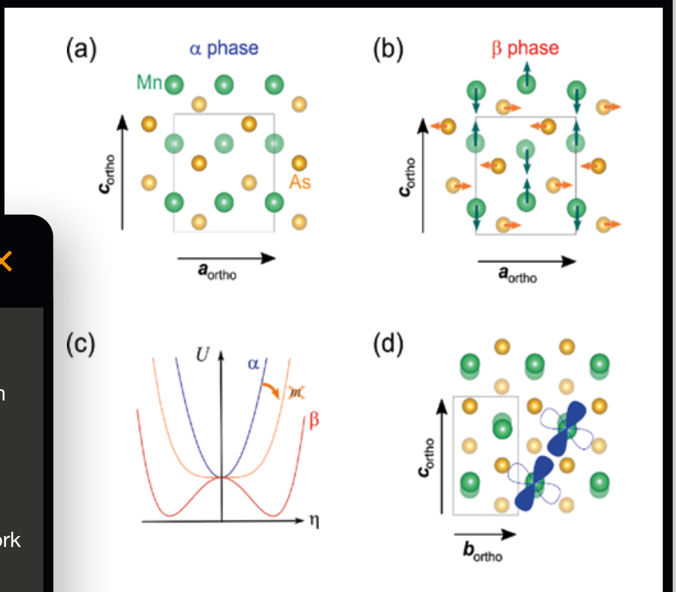

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Figure 1:
(a–b) MnAs crystallographic structure in the low-temperature ferromagnetic hexagonal α phase (a) and in the high-temperature orthorhombic β phase (b). Arrows in (b) indicate the displacement along the orthorhombic distortion η, associated with a soft phonon mode. (c) Schematic evolution of the potential as a function of η through the magnetostructural transition in the framework of the strong spin–phonon coupling scenario [5]. (d) Mn 3d-orbital hybridization in the hexagonal plane, according to the model of Ref. [6].

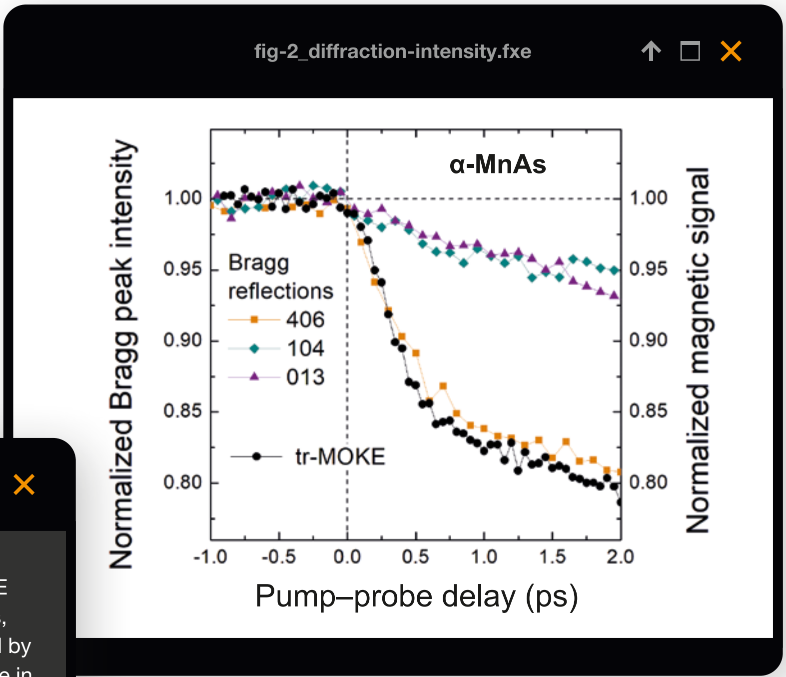

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Figure 2:
Time-resolved diffraction intensity measured at the FXE instrument for three of the selected α-MnAs reflections, compared to laser-induced demagnetization measured by magneto-optical Kerr effect. Mn and As sites contribute in phase to the structure factor for both the *406* and the *013* reflections, while only As contributes to the *104* reflection.

Because of its dramatic structural and magnetic changes with temperature (Figure 1), MnAs is a prototypical material for studying the strong coupling between crystal lattice and magnetism. The potential of MnAs for applications stems from a peculiar sequence of magnetostructural phase transitions, which have been studied for decades but are still not fully understood. Addressing the fundamental principles of how the crystal structures of these materials relate to their magnetic properties is a first step towards understanding how to control them and utilize them in concrete applications.

Recent theoretical studies have suggested two alternative mechanisms driving the transition between different magnetostructural phases in MnAs, one based on strong spin–phonon coupling in the ferromagnetic phase (phononic scenario) [5], the other based on changes in the electronic properties driven by a magnetization reduction of Mn atoms (electronic scenario) [6]. Both mechanisms impose characteristic signatures on the structural disorder accompanying the phase transition.

At the FXE instrument of the European XFEL, an international collaboration led by scientists of the Institut des NanoSciences de Paris in France used femtosecond X-ray diffraction to study the dynamics of structural modifications occurring in laser-excited MnAs. The FXE experiment was designed to help discern whether the phase transition should be described in the phononic or the electronic scenario, as proposed by theory.

The research team carried out time-resolved X-ray diffraction experiments at FXE on MnAs thin films, combined with laboratory-based magnetization dynamics measurements, with the objective of triggering the optically induced ultrafast demagnetization in MnAs while monitoring the structural changes on the same time scale, an approach already developed in previous experiments [7]. By choosing an appropriate set of Bragg reflections, the researchers could address the structural disorder dynamics along different crystallographic directions and discern whether they were involving both Mn and As sites equally, or Mn sites primarily.

The obtained results (Figure 2) indicate that the magnetic Mn sites are primarily affected, supporting the electronic scenario mentioned above, where magnetic excitations favour the bonding of Mn d-orbitals in the hexagonal planes (Figure 1d) providing the driving force for the orthorhombic distortion, with a decrease of the Mn–Mn distance and local antiparallel coupling of the Mn magnetic moments.

This study shows that combining measurements of magnetization and structural dynamics can shed light on the atomistic mechanisms in these fascinating materials. Beyond its fundamental interest, a better understanding of these mechanisms is valuable for the optimization of material properties, especially when the ultrafast dynamic response is of importance for applications, such as in magneto-acoustics and spintronics.

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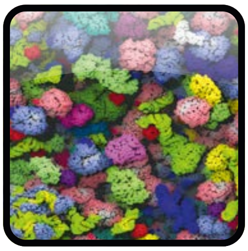
Investigating protein solution dynamics with MHz repetition rates



A novel experiment opens up the possibility of studying collective dynamics, providing insight for better drug design, delivery, and dosage.

Proteins carry out a wide range of important functions in our bodies. Knowledge about how they move around and through the crowded environments of our cells and tissues is key to understanding how they perform these crucial functions. Experiments exploring protein dynamics, however, often use samples that do not reflect the crowded and complex environments of the cell. At the MID instrument, scientists carried out X-ray photon correlation spectroscopy experiments to measure the nanoscopic structural dynamics of protein solution samples. The combination of this technique with the high repetition rate of the X-ray pulses generated by the European XFEL opens up the unique possibility of studying collective dynamics in protein solutions with high concentration, which is particularly interesting in the context of intracellular transport in eukaryotic cells and in drug design.

Catalysts, transporters, gatekeepers, and messengers—proteins carry out a vast range of different roles in our bodies. In addition to their structure, how they move through and interact and react with their crowded and complex environment impacts their function. Yet our understanding of the dynamics of processes, such as protein diffusion and transport in cells and tissues, is still lacking.

“Protein dynamics in crowded media, especially diffusion and transport, are essential for biological processes and cellular function,” explains Mario Reiser, scientist at Stockholm University in Sweden. A comprehensive knowledge of how proteins behave in these environments is especially useful for the design of new drugs. “When drugs enter our bloodstream, they bind to proteins that transport and distribute them around the body,” explains Christian Gutt, scientist at the University of Siegen in Germany. “How fast this happens is crucial information for understanding the time scale for a drug to be dispersed, but also, in the case of cancer drugs, how and when toxicity levels are reached as the amount of protein-bound drug increases in the bloodstream. A comprehensive understanding of the dynamics of these kinds of processes could lead to more effective treatments with fewer side effects.”

However, experimental work studying protein dynamics has, until now, primarily relied on techniques that either focus on single molecule properties or yield information on dynamics at larger length scales and longer time scales. “Many factors influence protein diffusion and transport within the crowded environment of our cells, including crowding by other molecules, local hydration, and water effects as well as temporary cluster formation with other proteins, which all slow down and hinder protein movement,” says Foivos Perakis from Stockholm University. Studies also show that the dynamics of proteins in crowded cellular spaces exhibit different behaviour patterns than those of other systems. All of these factors need to be taken into account for a full understanding of these systems.

“In highly concentrated environments, the dynamics differ significantly from that of a dilute system,” remarks Fajun Zhang, scientist at the University of Tübingen in Germany. “Clearly we lack information on the collective dynamics at length scales comparable to the dimension of the proteins and at time scales on the order of microseconds, where long-time diffusion acts,” he adds. “X-ray photon correlation spectroscopy, combined with the high repetition rates of the European XFEL, can access these time scales and, importantly, provide information on processes such as cluster formation.”

At the MID instrument of the European XFEL, Reiser, together with colleagues from around the world, employed low-dose X-ray photon correlation spectroscopy on antibody protein solutions containing immunoglobulin proteins (Figure 1). The experiment delivered a wealth of information and new insights, including how the diffusion

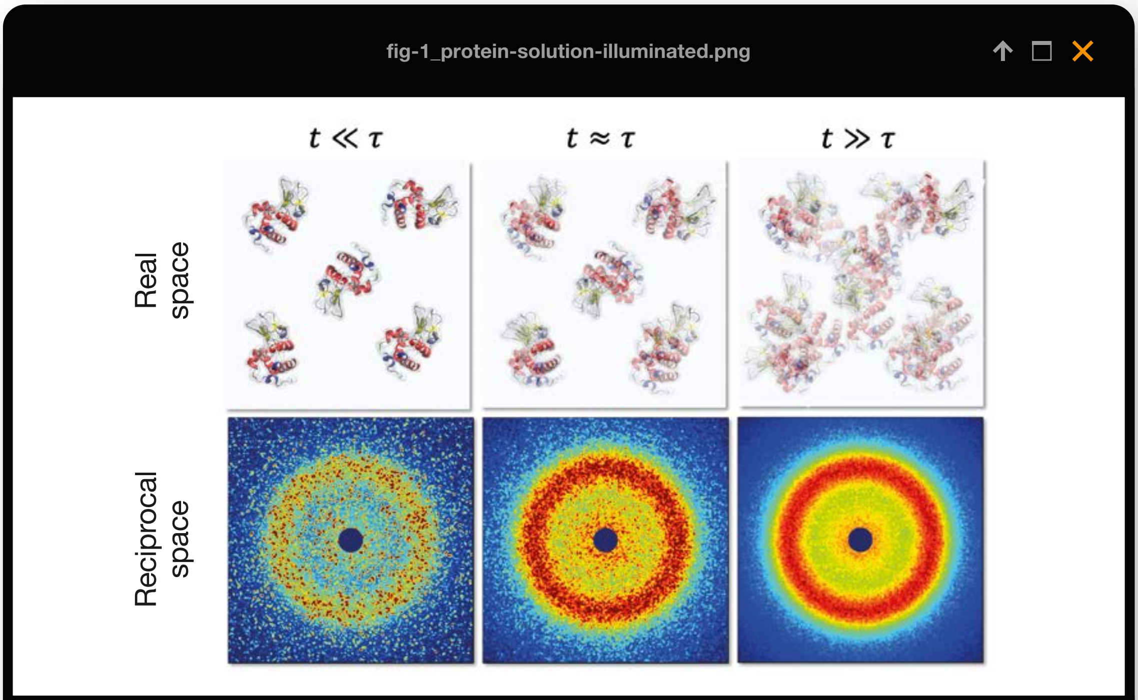


Figure 1:
Illuminating the protein solution with coherent X-rays gives rise to a grainy speckle diffraction pattern in reciprocal space. The protein dynamics are encoded in the intensity fluctuations of the speckles, which lead to a smearing out of the pattern when the measurement time (t) is larger than the relaxation time (τ) of the protein diffusion.

dynamics changed in relation to the dose rate and how cluster formation varied over time and space.

“This first protein X-ray photon correlation spectroscopy experiment at MHz repetition rates opens the door to investigating the microsecond-time-scale fast dynamics on microscopic length scales, which was previously inaccessible by other techniques,” says Anders Madsen, MID instrument group leader. “Protein dynamics on these time and length scales are closely related to protein–protein interactions that determine reaction speeds, protein function, aggregation, phase separation, and solution viscosity, with obvious implications for modern drug design and our understanding of various protein-related pathologies,” he adds.

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Towards faster and denser data storage systems

X-ray scattering experiments reveal important insights into ultrafast excitation of magnetic materials, which shows promise for next-generation data storage solutions.

The amount of data being produced and consumed around the globe every day is growing exponentially, leading to an ever-increasing demand for faster, more energy-efficient, and denser data storage solutions. In hard drives, where magnetic materials are used for long-term and stable storage, bits of data are typically written to the drive using a local magnetic field. For future generations of data storage systems, ultrafast excitation of magnetic materials by way of an optical or electrical pulse shows much promise as a faster method of writing data. However, the process of ultra-fast excitation of magnetic materials must be better understood at a fundamental level before it can be made commercially available. At the SCS instrument, an international team of scientists performed time-resolved X-ray scattering experiments on magnetic multilayered samples, revealing important new insights into the process of ultrafast excitation for energy-efficient bit writing and data stability.

In a report published by the Global DataSphere from the International Data Cooperation in May 2020, more than 59 zettabytes (ZB) of data were forecast to be generated and consumed that year across the globe [1]. In 2021, an estimated 74 ZB were produced; in 2024, this is projected to reach around 149 ZB [2]. As the amount of data grows exponentially, there is an increasing demand on industry to develop faster, more energy-efficient storage solutions, with increased storage density and faster writing speeds.

In the current generation of hard drives, a local magnetic field is commonly used to write data to the drive in the form of binary digits ("0"s and "1"s), or bits. The bits are laid down as magnetic field switches. The speed with which data can be written is limited, however. Recent studies have shown that an alternative approach using ultrafast optical [3, 4] or electrical [5] excitation can achieve the same result. Due to the ultrashort pulses needed, this method of magnetization switching promises to reduce bit-writing times significantly [5].

"Ultrafast excitation could be a real solution in the quest for developing faster and more efficient data storage systems, including cloud services and artificial intelligence solutions," says Serguei Molodtsov, scientific director at European XFEL. "However, before ultrafast excitation can be made commercially available, this process must be understood on a fundamental level."

Previous studies have been able to reveal important details of how this process works, such as identifying the pathways by which the magnetization recovers order, including momentum transport mediated by the material's composition [6] and conservative magnon processes at the nanoscale influenced by spin superfluidity [7].

"It is clear that, for further progress, there must be a detailed understanding of how the magnetization evolved spatially," explains Nanna Zhou Hagström, a Ph.D. student based at Stockholm University in Sweden. "This is precisely what we set out to investigate at the European XFEL, where the high-repetition-rate, bright X-ray flashes now give us the possibility of exploring these fast dynamics with nanoscale and femtosecond resolution."

At the SCS instrument of the European XFEL, Zhou Hagström, together with a large group of scientists from around the world, performed time-resolved X-ray scattering by exciting samples consisting of alternating layers of cobalt-and-iron alloy and nickel (CoFe/Ni), grown on a silicon membrane. The experiments used a femtosecond optical pulse to induce dynamics in the magnetization, which were subsequently recorded by means of a series of time-delayed X-ray scattering patterns [8].

The CoFe/Ni multilayers exhibit perpendicular magnetic anisotropy, which favours magnetization arrangements, or domains, oriented at 90 degrees to the film's plane. Magnetic multilayers with perpendicular magnetic anisotropy are commonly used in industry due to the increased bit density and stability they provide.

fig-1_magnetization-patterns.nano

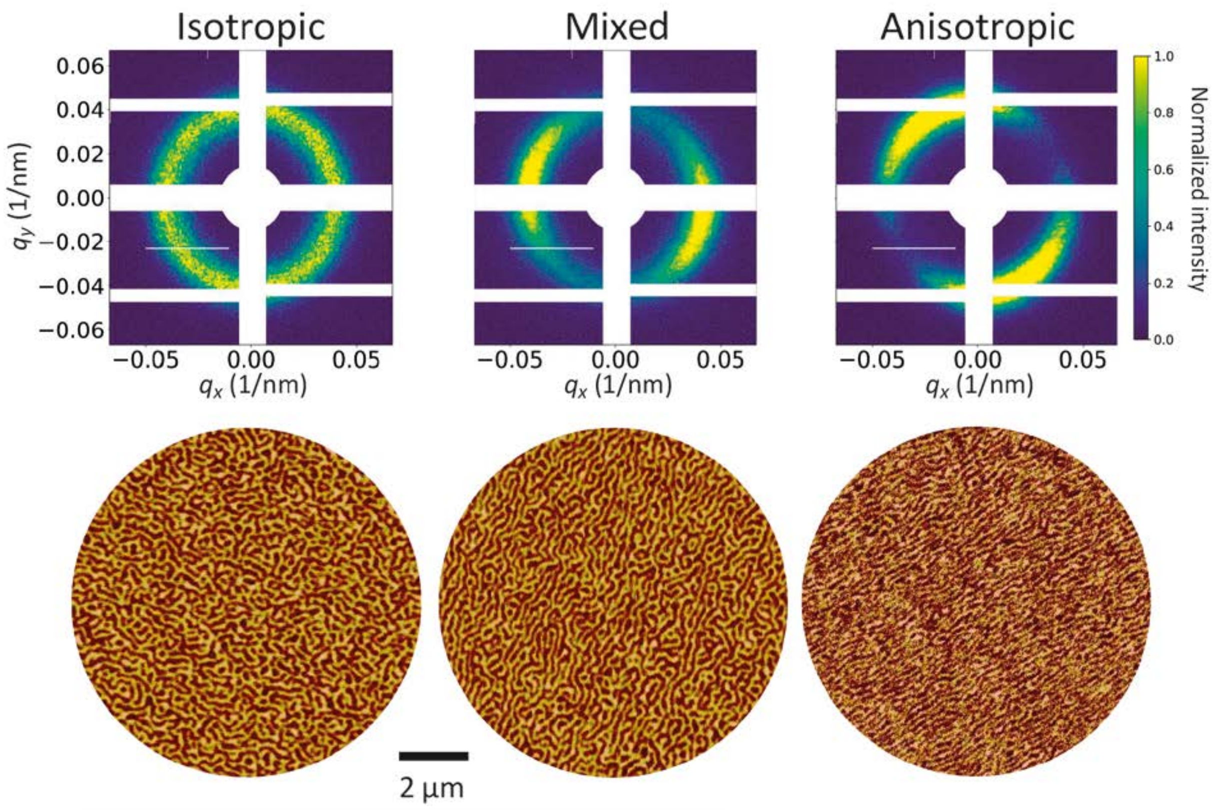

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Figure 1:
Nanoscale magnetization patterns and their equilibrium X-ray scattering collected at the SCS instrument

For their experiment at the European XFEL, the team studied different domain arrangements to get a better picture of the ultrafast spatial changes of the domains in the material. “We were able to grow and study a variety of magnetic domain arrangements, ranging from labyrinth domains exhibiting isotropic—that is, uniform—scattering to preferentially striped domains exhibiting anisotropic scattering, as well as mixed states with both features present,” explains Thomas J. Silva from the National Institute of Standards and Technology (NIST) in the USA, who designed the experiment. The symmetries of each domain were then revealed in the X-ray scattering patterns the team collected (Figure 1).

The scientists were able to reconstruct how the scattering profile changed over time, even disentangling the isotropic and anisotropic contributions to the scattering. “Anisotropic ultrafast spin dynamics is emerging as a key feature in materials where magnetic anisotropy is present in some forms, either in the domain structure, like in this case, or in the magnetocrystalline anisotropy,” says Stefano Bonetti from Stockholm University and Ca’ Foscari University of Venice in Italy, one of the senior authors of the work.

“While the mechanisms behind this observation remain to be explained, our results clearly demonstrate that the ultrafast response of domain patterns is symmetry-dependent,” says Ezio Iacocca from the University of Colorado, Colorado Springs, USA, who coordinated the data analysis. “By manipulating these symmetries in the ultrafast regime, it could be possible to unlock novel storage and computing schemes.”

“This study showcases a fascinating example of how symmetries can affect the properties of materials in a far-from-equilibrium setting,” says Andreas Scherz, group leader of the SCS instrument where the experiment was carried out. “In particular, this work will enable a more profound understanding of how angular momentum flows at picosecond time scales over much longer distances than those expected for ballistic electrons in a metallic alloy."

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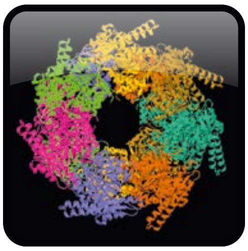
First single-particle imaging experiment at the European XFEL



A long-awaited breakthrough opens up the possibility of imaging individual biomolecules, for example to study the fast dynamics of proteins.

Exploring the structure of a single protein has long been a dream for structural biologists. However, it has never actually been demonstrated before now. In a recent experiment at the SQS instrument, scientists were, for the first time, successful in collecting data from a ribosome and a protein. The experiment proves that single-particle imaging can be used to explore the structure of biomolecules, providing an additional tool to the structural biologist's toolbox for studying fast dynamics of proteins.

Being able to determine the structure and dynamics of single biomolecules with X-rays has long been the ultimate goal for many biologists. "Single-particle imaging was presented as a major use case for the construction of the first X-ray free-electron lasers," says Filipe Maia from Uppsala University in Sweden, "and for good reason—the combination of ultrafast pulses and the ability to collect data from a single particle at a time could make it possible to study very fast dynamics in proteins, which is currently out of reach with today's methods." [1].

Even using the extremely bright X-ray flashes available at X-ray FELs, however, the results to date have been underwhelming, with the smallest objects studied so far being cells and viruses [2, 3]. "A major reason for this is that the diffracted signal from something as small as a single protein is still very weak compared to the diffraction from the gas that makes it into the vacuum chamber together with the injected sample," explains Tomas Ekeberg, also from the Uppsala team.

In X-ray single-particle imaging experiments, isolated molecules, ideally proteins, are injected into the X-ray beam. The intense X-ray pulse will quickly destroy the sample, but, since the damage processes are slow compared to the extremely short femtosecond X-ray pulse, the diffracted light and respective diffraction pattern collected by the detector will still represent the mostly undamaged structure [4]. However, scientists have so far been unable to generate any experimental verification of whether the principles of injection and outrunning the damage processes work for such biomolecules.

A recent experiment at the SQS instrument of the European XFEL attempted to remedy these problems by performing the experiments at a much lower photon energy than typically used. "By using a photon energy of 1200 eV, we could dramatically increase the scattering from the sample," explains Maia, who led the experiment. "The downside, however, is that the maximum achievable resolution decreased."

The first sample the scientists tried was a bacterial ribosome, a very large macromolecular complex responsible for translating DNA into proteins. It has a total weight of 2.7 megadaltons (MDa) and a diameter of around 20 nm. "We felt that a sample as large as the ribosome will undoubtedly scatter a lot and is therefore suitable for this proof-of-concept experiment," explains Ekeberg. "We recorded a total of 92 000 patterns and, from these, 1071 were identified as having a signal above the background level."

To verify their data, the scientists used an automatic size identification algorithm that compared the diffraction pattern with that of a sphere, thereby identifying the diameter that gives the best agreement with the experiment data (Figures 1 and 2). "We can see a large peak centred around the expected size of 20 nm, indicating that the majority of our measured particles are indeed ribosomes," says Ekeberg. This agrees with results from an identical control experiment run on the same sample under the same injection conditions.

The second sample studied was much smaller, the chaperone protein GroEL, with a molecular weight of 800 kDa and a diameter of 14 nm [5]. From the 225 000 X-ray pulses and corresponding detector readouts, only one pattern could be identified to originate from a GroEL fig-1_ribosome-size.xls

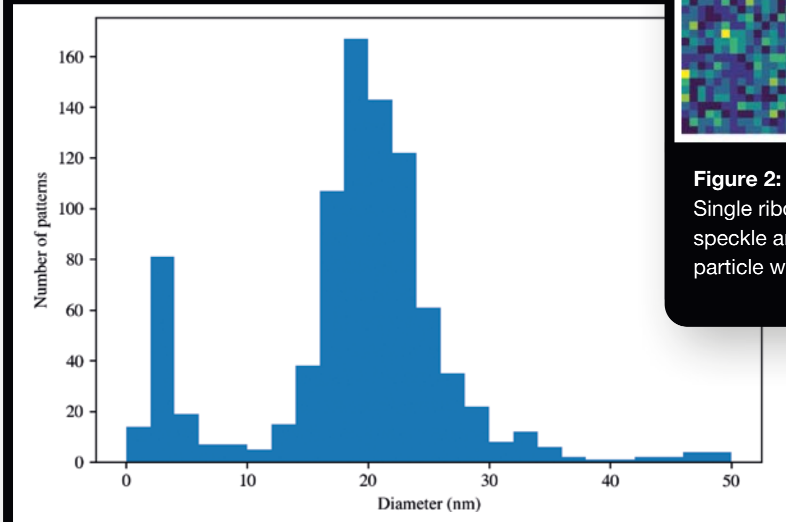


Figure 1:
Histogram of ribosome size. There is a large peak around the expected size of 20 nm. The smaller peak below 10 nm most likely comes from salt aggregates from the buffer solution.

fig-2_ribosome-pattern.png

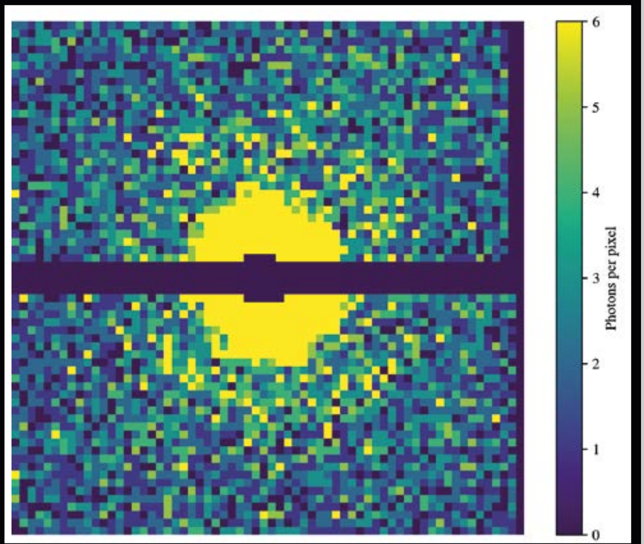


Figure 2:
Single ribosome diffraction pattern. The shape of the central speckle and first diffraction ring is consistent with a spherical particle with a size of 20 nm.

molecule with high certainty (Figure 3). “With only one pattern, we have to resort to other methods to verify that the pattern is indeed from the expected protein,” says Ekeberg. “Even though the pattern matches an object of the correct size, size alone is not enough to rule out water droplets or salt aggregates.” However, while the ribosome is a fairly spherical complex, the barrel-like shape of GroEL makes it distinctly non-spherical even at low resolutions (Figure 4). This deviation can be seen in the diffraction pattern as the first ring is broken up into four distinct speckles. This is consistent with a side view of the barrel-like protein.

“This initial analysis suggests that we have detected diffraction both from the very large ribosome complex and from the significantly smaller GroEL,” says Maia. “These findings finally give us the proof-of-concept for imaging single proteins using this method and show that the proteins survived the injection process and indeed made it to the X-ray beam.” He adds: “This is a long-awaited and exciting milestone on the path towards ultrafast structure determination from isolated particles.”

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fig-3_GroEL-pattern.png

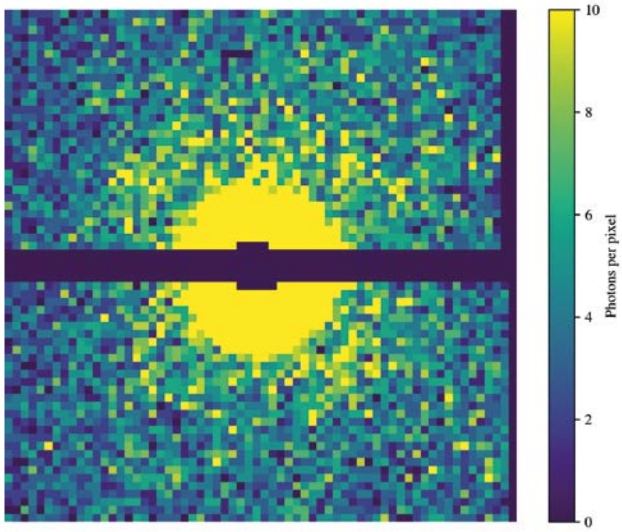

Figure 3:
Single GroEL diffraction pattern. The pattern shows deviation from rotational symmetry that is consistent with that of a barrel-like shape with the size expected for GroEL.

fig-4_GroEL-structure.tif

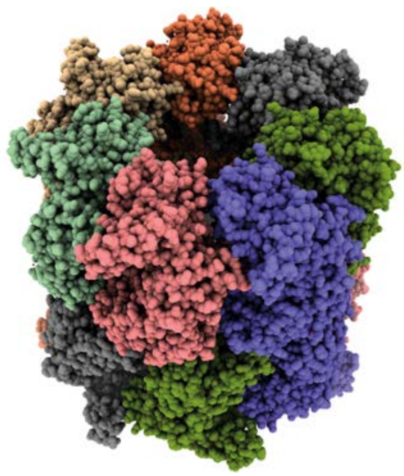

Figure 4:
Structure of GroEL. The structure is barrel-shaped, which makes this protein distinctly non-spherical even at low resolution.

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An explosive photoshoot

Groundbreaking Coulomb explosion imaging experiment paves the way for filming chemical reactions in single small molecules.

From photosynthesis to processes within our eyes—many key reactions in our world are triggered by light. Capturing details of these fast photochemical reactions as molecular movies could help provide crucial knowledge for the development of new medical therapies, sustainable energy solutions, and materials. Using a method known as Coulomb explosion imaging, which utilizes the capabilities of the European XFEL to explode molecules, an international team of scientists has successfully captured images of iodopyridine molecules at atomic resolution. The experiment at the SQS instrument paves the way for producing movies to gain key insights into fast chemical reactions.

Exploding a photo subject in order to take its picture? A research team at the European XFEL employed this "extreme" method to take pictures of complex molecules. The scientists used the ultrabright 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. "Thanks to the European XFEL's extremely intense and particularly short X-ray pulses, we were able to produce an image of unprecedented clarity for this method and the size of the molecule," reports Rebecca Boll from the SQS group at European XFEL, principal investigator of the experiment and one of the two first authors of the publication in which the team describes their results [1]. Such clear images of complex molecules have not been possible using this experimental technique until now.

The images are an important step towards recording molecular movies, which researchers hope to use in the future to observe details of biochemical and chemical reactions or physical changes at high resolution. Such films are expected to stimulate developments in various fields of research. "The method we use is particularly promising for investigating photochemical processes," explains Till Jahnke from European XFEL and the Goethe University Frankfurt in Germany, who is a member of the core team conducting the study. Such processes, in which chemical reactions are triggered by light, are of great importance both in the laboratory and in nature, for example in photosynthesis and in visual processes in the eye. "The development of molecular movies is fundamental research," Jahnke explains, hoping that "the knowledge gained from them could help us to better understand such processes in the future and develop new ideas for medicine, sustainable energy production, and materials research."

In the method, known as Coulomb explosion imaging, a high-intensity and ultrashort X-ray laser pulse knocks a large number of electrons out of the molecule. Due to the strong electrostatic repulsion between the remaining, positively charged atoms, the molecule explodes within a few femtoseconds. The individual ionised fragments then fly apart and are registered by a detector.

"Up to now, Coulomb explosion imaging was limited to small molecules consisting of no more than five atoms," explains Julia Schäfer from the Center for Free-Electron Laser Science (CFEL) at DESY, the other first author of the study. "With our work, we have broken this limit for this method." Iodopyridine (C_5H_4IN) consists of 11 atoms (Figure 1a).

The film studio for the explosive molecule images is the SQS instrument at the European XFEL. A cold target recoil ion momentum spectroscopy (COLTRIMS) reaction microscope (REMI) developed especially for these types of investigations applies electric fields to direct the charged fragments onto a detector. The location and time of impact of the fragments are determined and then used to reconstruct the momentum—the product of mass and velocity—with which the ions hit the detector (Figures 1b and c). "This information can be used to obtain details about the molecule, and, with the help of models, we can reconstruct the course of the reactions and processes involved," says DESY researcher Robin Santra, who led the theoretical part of the work.

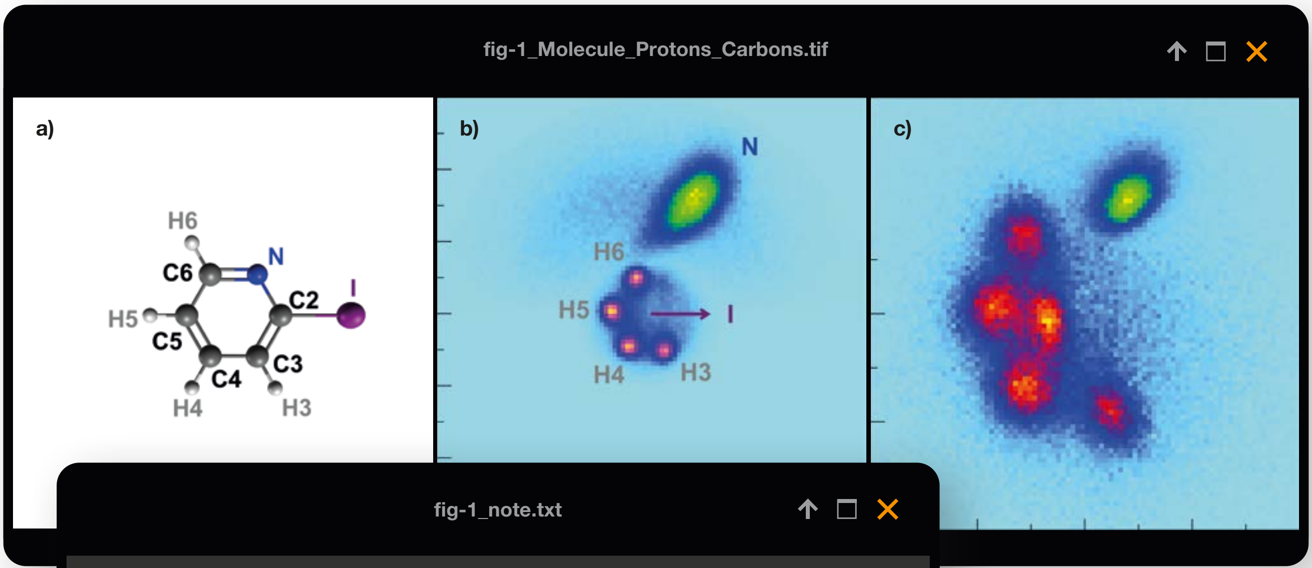

fig-1_note.txt

Figure 1:
(a) Structure of iodopyridine. The ring is formed by carbon atoms (grey) and a nitrogen atom (blue). The iodine atom (violet) is on the outside of the ring. (b) In this Coulomb explosion imaging result, the team concentrated on the hydrogen atoms (violet). The shape of the ring can be clearly seen because the hydrogen atoms are the first to be emitted from the molecule due to a charge-up of the ring atoms. The heavier nitrogen atom is emitted later in the process, when more charge has accumulated. As a result of the stronger repulsion, its momentum is larger than that of the hydrogen atoms. (c) The Coulomb explosion image of the molecule shows the carbon atoms (red) and the nitrogen atom (green) in detail. The ring appears distorted because the detector does not register a direct image but the momentum of the fragments from the explosion. The iodine atom is not displayed as it defines the horizontal axis of the momentum space coordinate system.

Coulomb explosion imaging is particularly suitable for tracking very light atoms, such as hydrogen, in chemical reactions. The technique enables detailed investigations of individual molecules in the gas phase and is therefore a complementary method for producing molecular movies, alongside those being developed for liquids and solids at other European XFEL instruments.

"We want to understand fundamental photochemical processes in detail," says Jahnke. "In the gas phase, there is no interference from other molecules or the environment. We can therefore use our technique to study individual, isolated molecules." Boll adds: "We are working on investigating molecular dynamics as the next step, so that individual images can be combined into a real molecular movie, and have already conducted the first of these experiments."

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Highlights from FEL source R&D

Interdisciplinary collaboration for novel scientific applications

The FEL R&D virtual group is a collaborative and interdisciplinary team of scientists and engineers from different groups at European XFEL and DESY committed to improving the FEL sources and developing new FEL modes at the European XFEL. In 2021, the group greatly improved the capabilities of the FEL sources through R&D activities and by providing these new features for user experiments. The group achieved outstanding results in the realization of short pulses, multiple-colour two-pulse schemes, frequency mixing, higher photon energies, seeding, and timing stability. R&D studies of interesting questions in FEL physics and their practical applications in experiments are the foundation for novel scientific applications at the European XFEL.

Different scientific applications require X-ray pulses with specific properties. For example, to study changes in electronic states happening on time scales of a few femtoseconds or faster, X-ray pulses of similar or shorter duration are needed. In 2021, the FEL R&D group investigated methods to produce X-ray pulses on these time scales without the need for additional hardware. Consequently, special bunch compression schemes were used to actively control the FEL pulse duration for both soft and hard X-rays. This, in combination with the control of radio frequency parameters for individual electron bunches, could lead to independent control of all self-amplified spontaneous emission (SASE) FEL lines.

fig-1_SASE3-example-sequence.pdf

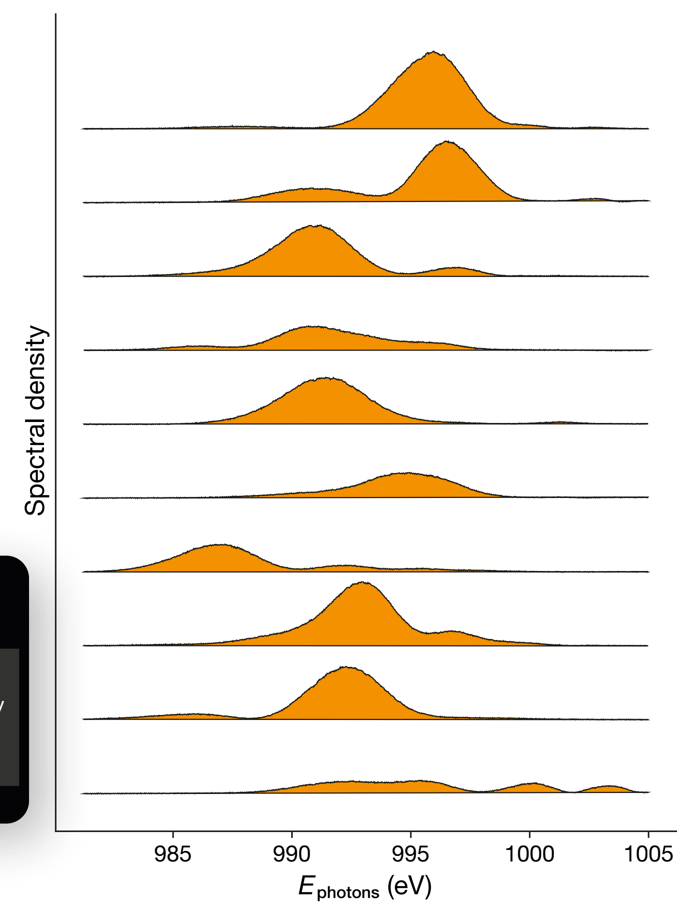

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Figure 1:
Example of a sequence of spectra from 10 successive X-ray pulses obtained at SASE3 at around 1 keV photon energy, corresponding to femtosecond-level pulse durations

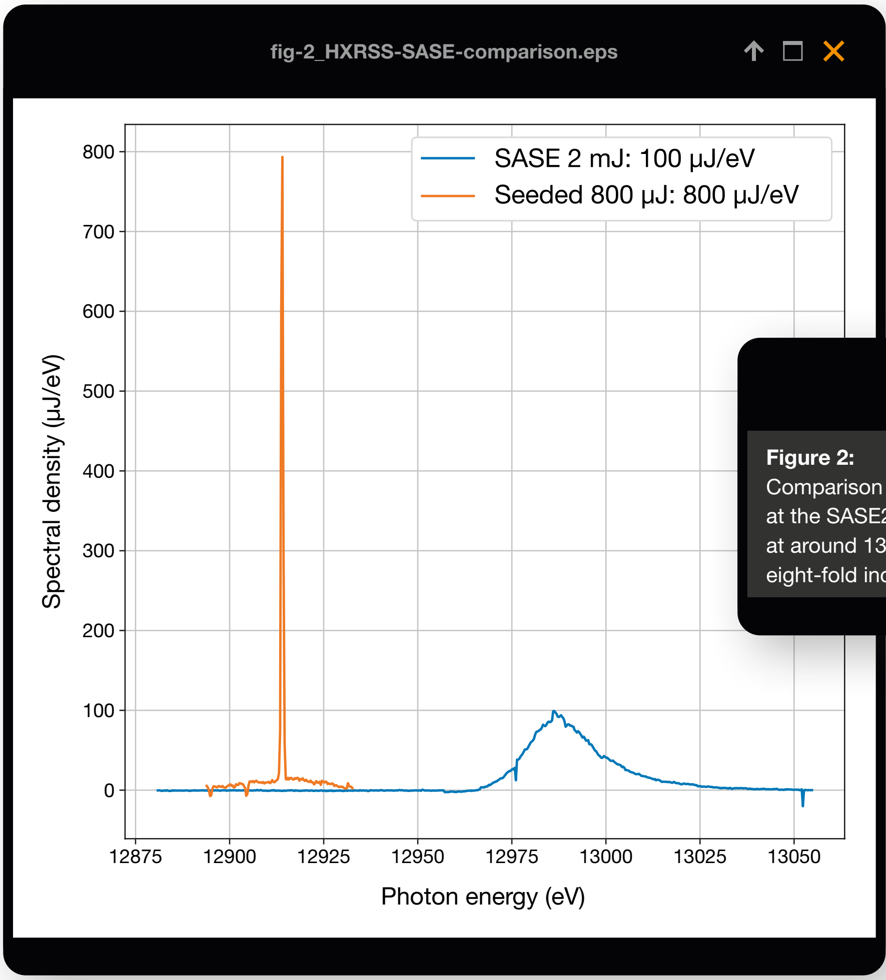

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Figure 2:
Comparison of HXRSS and SASE spectra measured at the SASE2 FEL, averaged over 1000 X-ray pulses at around 13 keV photon energy, demonstrating the eight-fold increase in spectral density.

In these studies, the group was able to provide sub-10 fs pulses at the SASE2 FEL, while, at the same time, SASE1 and SASE3 were operated for users with the nominal pulse duration of around 30 fs. At SASE3, an increased dispersion was introduced on the electron beam. As a result, only a selected part of the electron bunch travelled on a straight orbit through the undulator and had a higher electron density, and the duration of soft X-ray pulses at 1 keV photon energy was reduced to the femtosecond level with pulse energies at the 500 µJ level. This resulted in a fraction of the delivered SASE FEL pulses showing single spikes (Figure 1).

At SASE3, the group also tested, for the first time, the generation of X-ray pulses with expected durations in the sub-femtosecond range through harmonic conversion [1]. Starting from few-femtosecond-long X-ray pulses at 675 eV photon energy, obtained by means of non-linear compression in a first part of the undulator, the scientists observed fourth-harmonic pulses at 2.7 keV photon energy generated in a second undulator part, with single-spike spectra measured for about 1% of the pulses. High-gain amplification allowed for pulse energies on the 10 µJ level.

A second example of studies concerned the provision of multiple pulses from a single electron bunch, with different photon energy and delay between them. Using additional bunch compression parameters, the group could increase the stability of two-colour operation and allow for negative X-ray pump–probe delays at SASE3, as demonstrated already in 2020 and characterized using the time diagnostic tools at the SQS instrument. This capability was then used in two successful user experiments at the SQS and SCS instruments.

Two-colour pulse studies were also performed at SASE2 using the second magnetic chicane, designed with both hard X-ray self-seeding (HXRSS) and two-colour applications in mind. In the hard X-ray range, the group was able to show tuning of the delay between the pulses and of their wavelength at pulse energies of several hundreds of microjoules. This new capability will be made available to users in 2022.

HXRSS is an example of advanced bunching manipulation that provides an X-ray beam with a reduced bandwidth $\Delta E/E \approx 10^{-4}$ and improved spectral density (Figure 2). HXRSS was successfully delivered at 9 and 13 keV photon energy to two user experiments at the MID instrument, analysing the dynamics in a crystal lattice with up to 300 bunches per train, and to a polarimetry experiment at HED, with up to eight times stronger peak intensity (up to 800 μJ/eV) than provided by the SASE process.

Advanced bunching manipulation was also exploited in frequency-mixing experiments at SASE3 [2]. Two frequencies were generated in a first part of SASE3 in alternating *K* parameter configuration, and, upon slight compression, the difference frequency was radiated and amplified in a final third part of SASE3. Pulse energies on the millijoule level were produced, depending on the length of the radiator part, with photon energies between 500 eV and 1.1 keV. In the near future, the freshly installed APPLE-X undulator could be used as radiator, which would allow for extending the SASE3 range to lower photon energies.

The development of novel capabilities was accompanied by significant improvements in the standard SASE mode of operation. In particular, high-repetition-rate pulses with pulse energies of a few 100 μJ at the record-high photon energy of 30 keV were available at SASE2, and pulses of about 800 μJ at 24 keV were used for first user experiments at SASE1. At SASE3, a unique combination of high electron energy (16.3 GeV) and special bunch compression allowed the group to achieve, at 1 keV photon energy, single pulses of more than 15 mJ pulse energy, a mode that needs to be further studied before delivery to users.

During setup and operation of these special modes, diagnostics were crucial. Key roles were played by the spectrometers—the SASE2 high-resolution hard X-ray single-shot (HIREX) spectrometer and the SASE3 monochromator—and the X-ray gas monitors [3, 4].

Using pulse-resolved timing diagnostics, the group was able to demonstrate that the improved short-term stability achieved by the application of electron-beam-based feedbacks was, to a large extent, preserved during the FEL process and following photon beam transport (to the SPB/SFX and SQS instruments), with a typical photon arrival time jitter of 10 fs (RMS) at a bunch charge of 100 pC and 6 fs (RMS) at 250 pC (measurement resolution: beam arrival time monitors <5 fs RMS, photon arrival time monitors <3 fs RMS).

Further development of these and new techniques will keep the group busy for years to come. The group members expect that their collaboration, spanning instruments and support groups, will continue to develop, based on the shared values of European XFEL.

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European XFEL Data Operation Centre

The Data Operation Centre (DOC) is a single entry point to support services provided by the European XFEL Data Department. Established in early 2021, the DOC has had a positive impact on operational efficiency and data quality at the facility. Rotating shift crews and data run coordinators (DRCs) oversee data services important for X-ray operation, including IT, data acquisition, analysis infrastructure, the control system, and detector systems. The DOC has led to enhanced communication and knowledge transfer both within the Data Department and with the scientific instrument groups and has significantly reduced the support load on individual groups. This article outlines the motivation behind the creation of the DOC and summarizes the experience gained from one year of operation.

The Data Department is tasked with providing data-related services for European XFEL, facilitating the acquisition and analysis of high-quality data for the scientific user community. These services include programmable logic controllers (PLCs), which provide the interfaces to most instrument hardware, such as vacuum or motion systems, and the Karabo control system, which exposes user interfaces and integrates cameras, custom digitizers, or humidity sensors. Automated procedures improve efficiency, while state-of-the-art X-ray detectors acquire up to 8000 images/s in 4.5 Mfps bursts and and output data at up to 15 Gb/s, or 1 PB of data in a few days. A data acquisition system and databases store persistent data and make them explorable, and they feed calibration and analysis services that enable near-real-time feedback to scientists.

fig-1_DOC-workstations.DNG

fig-1_note.txt

Figure 1:
The European XFEL Data Operation Centre. The two workstations for the shift leader and the deputy are visible in the front. In the back, four large screens can be flexibly configured to monitor the services provided by the Data Department.

Efficient and stable operation of data services has a high impact on scientific data collection; even relatively simple failures can delay experiments significantly. A detailed analysis of procedures at European XFEL revealed two main “time sinks” in the support of these services. First, in the event of a problem, instrument operators called various support lines to facilitate a solution. Due to the high complexity of data services at such a large FEL facility, this approach was inefficient without a good understanding of component interdependency. The second time sink involved small problems that often went unnoticed until they directly impacted measurements.

The DOC was created as a single, proactive point of entry for coordinated support to address these issues. Furthermore, the role of DRC was introduced as an escalation path for data services relevant to X-ray operation.

Now, when a problem arises, the DOC operator takes corrective action or identifies and contacts the *correct* support group. Additionally, the DOC can coordinate actions or even escalate priorities where more complex issues require multiple groups to resolve them.

Creating the DOC

Given the complexity and range of services to be covered, a task force was established as a first step to define, refine, and prioritize the facets and features of the DOC. An Agile process was chosen, tapping into the “hive knowledge” of the Data Department. The task force then split into three teams, responsible for hardware, monitoring tools, and documentation, respectively.

The task force made three noteworthy observations. First, they noticed that it is important to leverage existing solutions—the benefit of quickly creating content rather than first installing new tools outweighs the procedural compromises that existing tools might impose. Second, conscious technology choices avoid reliance on a few experts—choosing the then new InfluxDB time series database and its Grafana front-end as monitoring tools had people grow from a similar level of expertise, fostering collaborative learning. Finally, the task force noted that collaborative tools, such as virtual whiteboards, facilitate Agile meetings. Online surveys give feedback on whether goals are met.

Running the DOC

The DOC started operation in March 2021, at first supporting only a few experiments. Then, from May onwards, the DOC supported all experiments at all scientific instruments, on a schedule of two shifts a day.

Each incident handled by the DOC is logged. The logs allow for classification of support given, contact channels, proactiveness, and support duration. These statistics are enhanced with follow-up tickets made by the shift crews. Based on this information, a continuous improvement cycle for data services was established.

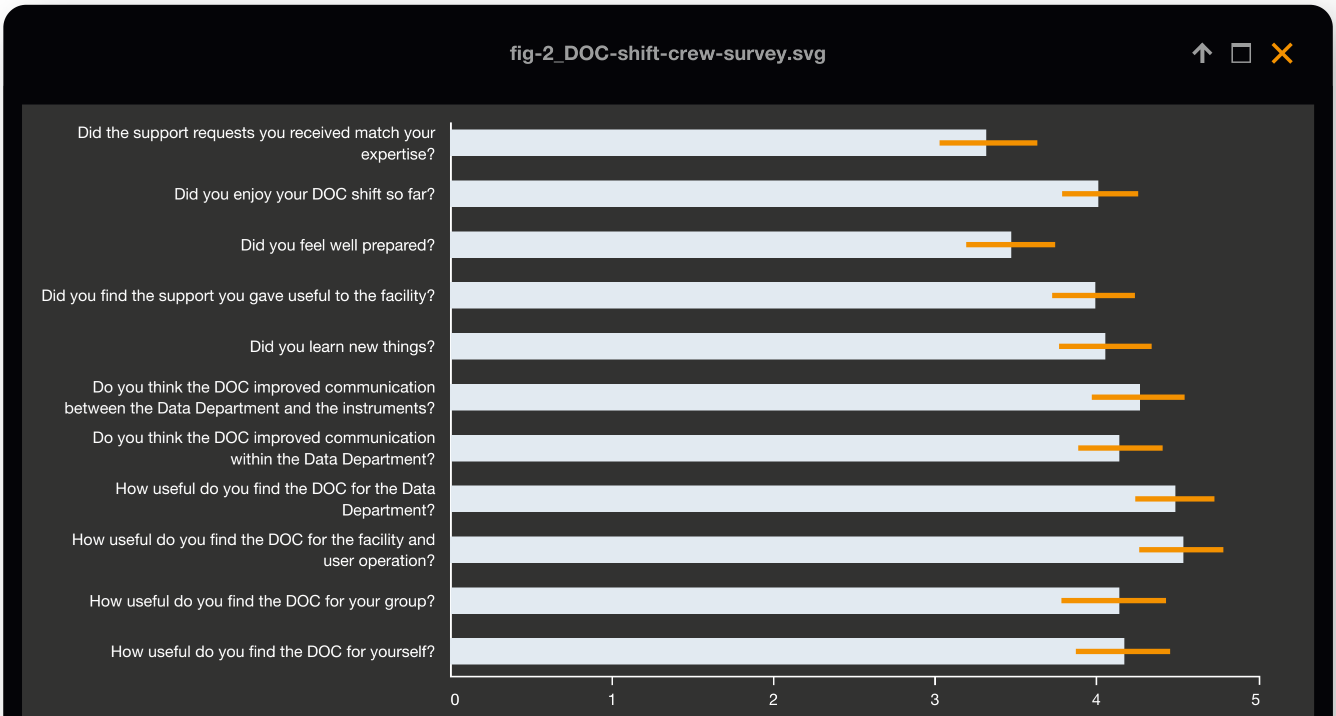

Figure 2:
Selected results from the DOC shift crew survey. Answers were on a scale from 1 (very negative) to 5 (very positive). The average feedback (grey bars) was generally very positive, with a small spread in answers (orange bars).

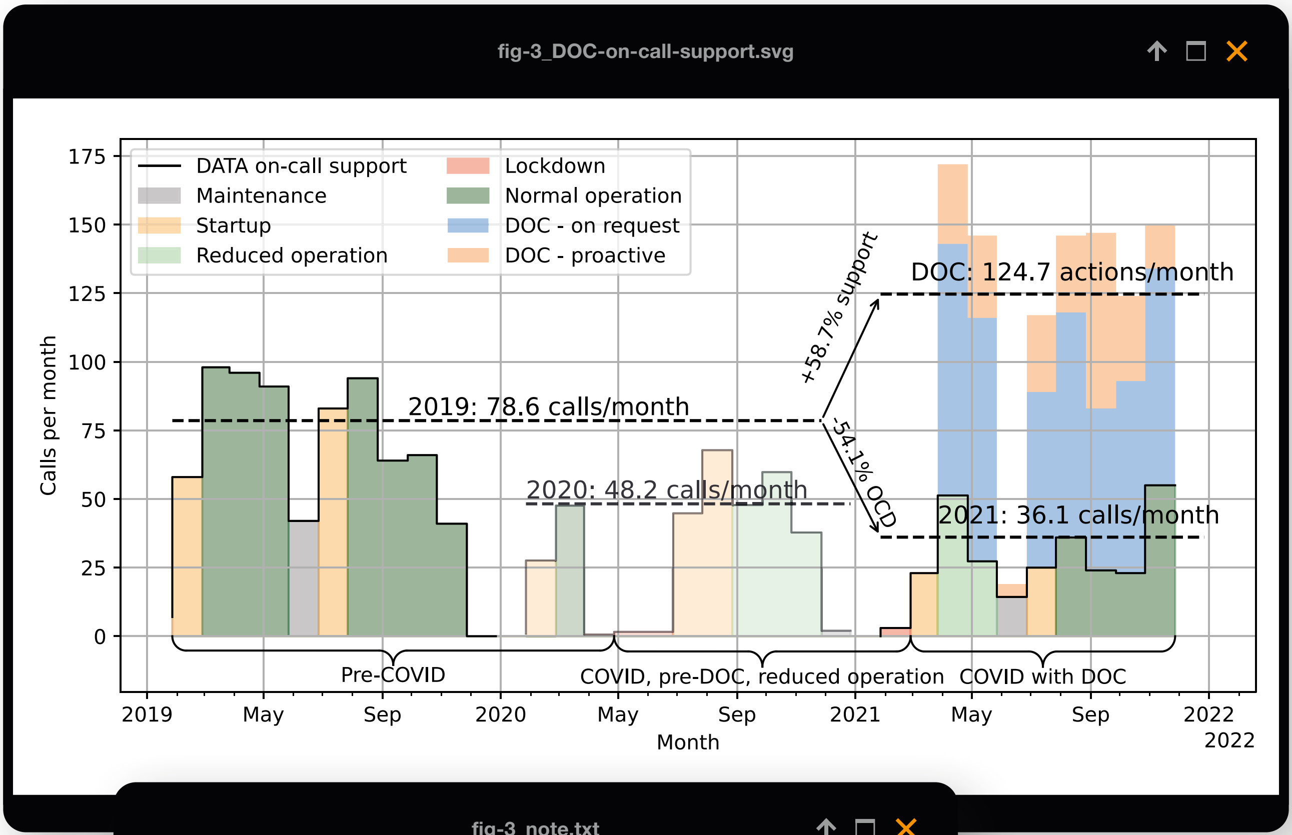

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Figure 3:
Monthly number of calls to on-call support in the Data Department. The DOC operation has led to a significant decrease in *ad hoc* support. The comparison is mainly between 2019 and 2021, as the operation was significantly reduced in 2020 due to COVID-19 measures.

Issues reported to the DOC vary greatly. Simple problems include, for example, an operator needing help to restart software that has been shut down[1]. Intermediate problems include misconfiguration of hardware and software[2], or supervision and support of recently added and extended service[3]. Complex problems include mechanical or electrical failures[4] or even large-impact failures involving multiple services.

In November 2021, staff members participating in the DOC and DRC shifts were asked to quantify their experience (Figure 2). A majority commented that the DOC had greatly improved communication within the Data Department and with the scientific instrument groups. Additionally, the cross-functional aspiration of the DOC works. People learn from colleagues with different experiences and expertise. At the same time, unplanned, *ad hoc* support requests have dropped significantly (Figure 3).

Summary

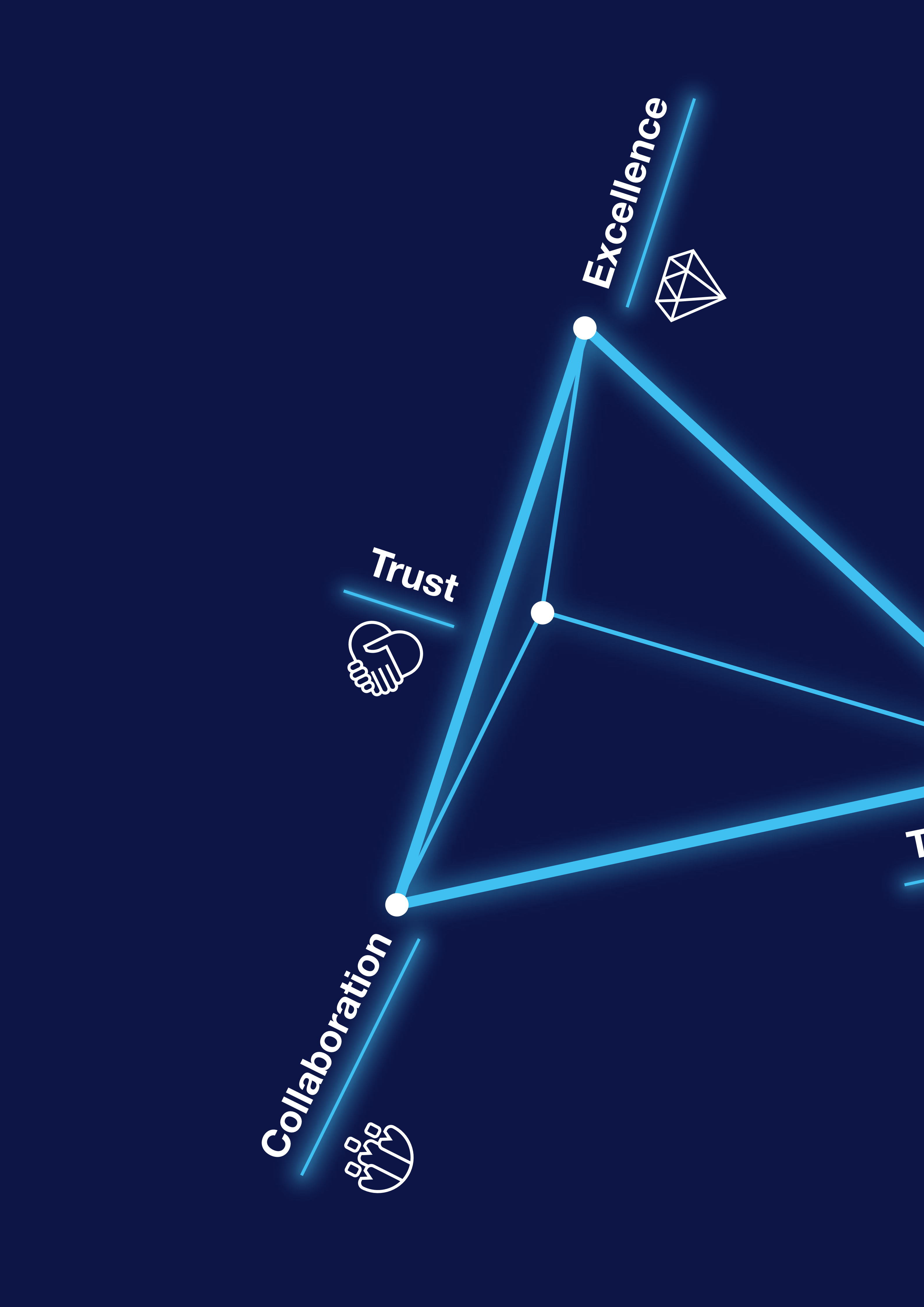
The DOC was introduced as the support entry point for services of the Data Department relevant to X-ray operation. The efficiency of support has increased and response times have shortened, which has increased the scientific output of the facility by increasing the beamtime available for scientific studies and by improving data quality. The concurrently introduced role of DRC has facilitated these efforts through a structured coordination and escalation path. Feedback from the scientific instrument groups is very positive, and surveys show that staff development, in terms of enhanced skills and responsibilities, works well in the context of the DOC.

1 Frequently, operators seek guidance from the DOC about whether restarting is the proper procedure.

2 Camera and detector settings are examples of topics on which the DOC recurrently advises.

3 Evolutionary online calibration services processing the full-rate output of megahertz detectors, for example, were closely monitored by the DOC after initial deployment.

4 Broken cables are a good example for when second-level support is usually requested from the DOC.


Excellence
Trust
Collaboration

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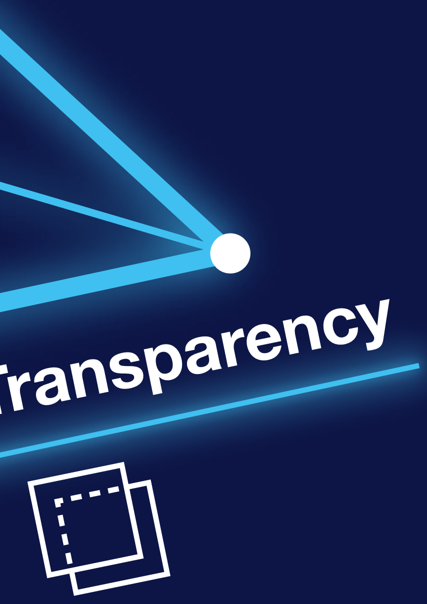
MAGAZINE

The European XFEL values—identified and defined by employees for employees



Values

“Collaboration”, “excellence”, “transparency”, and “trust”—these four values were identified and defined by staff members as core values for European XFEL. They are at the heart of the company mission and will help to build a supportive and highly motivated community within the company.

What is so special about the core values of “collaboration”, “excellence”, “transparency”, and “trust”? They are the result of a long bottom-up process. Rather than imposing top-down values on the company, the management board decided to have staff members themselves identify the core values.

Picking four core values from the vast lot of possibilities was hard work but an interesting process for all involved. The excitement generated by the process showed that these sought-after values are more than mere words. They will help define what the company is and what it stands for. They will send a message internally and externally about what is important to European XFEL. They will show what people expect from each other and from the users. And they will guide how we think and act.

To find out which values matter at our young research facility, a “Values” project team conducted a survey developed by a working group of “value ambassadors”. All were volunteers from a wide variety of groups, professions, and nationalities—the very diversity that makes European XFEL a special place to work. Later, a subgroup of 10 “culture change agents” was formed. This subgroup now meets regularly, discussing how to elevate awareness of the values and how to integrate them into work life.

Seventy percent of staff members took part in the “Values” survey, which identified aspects of company culture important to working together effectively. In evaluating roughly 2000 survey responses, the subgroup had to think about the overall aims of the company as well as the individual aims of every group and every staff member.

The questionnaire used pictograms to help participants identify their favorite values and weigh their impact. In the end, four core values—“collaboration”, “excellence”, “transparency”, and “trust”—were identified as most important.

fig-1_workshop-01.JPG

fig-1_note.txt

Figure 1:
Culture change agents workshop—defining priorities for each value

fig-2_XFEL-values.ppt

COLLABORATION
We collaborate at all levels.

We listen and collaborate in order to contribute to our common purpose.
We are responsible for what we do and reflect on how we act.

EXCELLENCE
We aim to be excellent where it matters.

We support and encourage everyone to be the best they can.
We strive to deliver on our mission to operate and grow a world-class science facility.

TRANSPARENCY
We value transparent processes and decisions.

We communicate honestly and openly and we are encouraged to speak up and present our own views.
We have well defined-processes and roles and we agree on clear, transparent decisions.

TRUST
We value trust-based relationships that respect the expertise and roles of our staff.

We are committed to building a trusting environment and are empowered to act with courage and integrity.
We act with empathy, fairness, and respect and we value our diversity.

Figure 2:
The European XFEL values—identified and defined by employees for employees

"When we analysed all the statements in the survey, we made an interesting discovery," says Ruth-Rebekka Sang, who manages the "Values" project and coordinates the culture change agent subgroup. "We all have clear expectations of how we and our co-workers should behave as well as a clear sense of what motivates and drives us. This does not mean that we all have exactly the same values, but it does mean that we have common ground."

"It was a very positive process," says Adrian Mancuso, leading scientist at European XFEL and a member of the "Values" working group. The four values came from data. These were not suggested explicitly—they were distilled through the bottom-up evaluation process. Adrian, as a scientist, is especially excited about the "excellence" value. "This is honestly great. I am naturally attracted to it because I want to do great science. When users, collaborators, and staff members value excellence, it will enable the lab and everybody in it to work better."

Once everyone agrees on "excellence" as a core value, nobody will settle for second best but will work to achieve the extraordinary. A company that is committed to the highest standards and that constantly endeavours to exceed expectations will continuously improve in all areas of work.

Christina Schmidt, research assistant and one of the culture change agents, is especially excited about the "collaboration" value. "It sounds abstract, but I am sure it will improve everyone's work life." She asked her colleagues to do a value exercise. The team chose to work on one core value: "collaboration". Every team member had to rate, on a scale from 1 to 10, where they saw "collaboration". What was its role in the daily work process, what were blockers and enablers, and what could be done to "bring the value to life?" And in some cases, little changes already produced a fair amount of positive feedback.

Managing Director Nicole Elleuche, who is responsible for the "Values" project in the management board, says: "I am happy and thankful for those four values. We need them to develop a personality as a young company, and every single one plays an important role. I was surprised and proud that our staff picked 'collaboration'. I am especially proud when I can present 'excellence' as a core value. It shows what we are aiming at. 'Transparency' is something we have to work on. And 'trust' is the value that I talk about most."

“We now have to develop a common understanding of what the values mean for the company”, says Ruth-Rebekka Sang. “Values are not something you just say. They are something you do. So, it is up to each staff member to turn our values into action. The goal is to create more effective and efficient ways of working. Therefore, it is important to find out what we can do better and how. Together with the culture change agents, we will develop a value action plan, step by step. We will strive to get every staff member pulling in the same direction at the same time.”

Taking the value “trust” as an example, European XFEL wants roles and responsibilities to be clearly defined and decisions to be taken according to responsibilities. In the medium and long term, this is expected to lead to streamlined processes and prudent management of resources.

Knowing that “trust” is accepted as fundamentally important for everyone will initiate a change in the daily work of the company’s leaders, says Nicole Elleuche. “There will be no need to discuss a proposal extensively if the leaders are trusted to know what they are doing.”

“Transparency”, “trust”, “excellence”, and “collaboration” will also be essential parts of the recruiting process, from start to finish. Attracting candidates who align with these values will increase the odds of a successful hiring process.

Studies show that companies with strong company values perform better and have more customer and employee satisfaction. Mission-driven organizations are on the rise, and values play an essential role. They help to build a strong company culture, align teams, and help them to make the right decisions.

“Having those values has two great benefits,” Christina Schmidt says. “They will enable us to do better science, and they will help us to create a warmer and more supportive workplace. I hope it will improve the work life of every single employee.”

There is no hierarchy of values. Although each of our values—“trust”, “excellence”, “collaboration”, and “transparency”—emerged by itself, all four are inter-connected and dependent on one other.

fig-3_workshop-group.JPG

Building and maintaining a positive cooperative relationship with co-workers and users needed for collaboration means that you have to pursue an open, communicative culture in which individuals are encouraged to offer suggestions for improvement. That is where trust comes in. Offering suggestions, sharing doubts, bringing up issues, proposing solutions, and communicating shortcomings will happen only when you can trust that you will be treated fairly.

Trust is not just about acting responsibly when nobody is looking. It is about constructive, candid communication, especially related to errors. It is about integrity, doing the right thing, acting truthfully and honorably. Building trust requires confidence, faith, patience, effort, and transparency.

Being transparent means sharing information, being honest, having no tolerance for hidden agendas or aggressive behaviour. It means communicating and making understandable why you do what you do. Transparency breeds trust. When all these values come together, they help make excellent science happen.

That is also how the User Organization Executive Committee puts it: “We were happy to see that these values were identified in a bottom-up process by a representative cross section of European XFEL staff, and we appreciate that the user community will be informed and involved at an early stage.”

However, it will take time, resources, and a lot of work to establish the values, to fill them with life and meaning, and to integrate them into every process, every group, every day. “We are aware that we are not yet there, but rather at the very beginning,” says Nicole Elleuche. “The process will need continuous attention and care, much like the cultivation of a plant. There are no simple instructions for our future growth and success; however, we are convinced that, if we nurture our values together, they will help us flourish!”

Jutta v. Campenhausen

fig-3_note.txt

Figure 3:
Our individual culture change mission statements — together we grow!

Factsheet 2021

Users

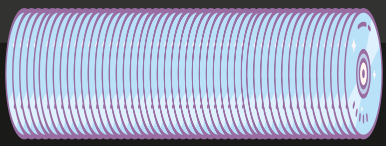
User experiments	Individual users	X-ray delivery to users
44	702	4664 h

Users on site	Ph.D. students among users
220	138

Electron and X-ray beams

Number of electron bunches per second: **27 000**	Diameter of the electron beam: ca. 50 µm (human hair)	
Number of SASE undulators running in parallel: **3**	Time of flight of an electron from the injector to the dump: **10 µs** (1/100 000 seconds)	
Minimum wavelength of the X-ray flashes: **0.04 nm** (30 keV)	Smallest focus of the X-ray beam: **11 nm**	Highest number of X-ray flashes per second: **21 000**

Data 2021



PB raw data collected: 18.1 PB
(= 18 100 TB, 18 100 000 GB, 18 100 000 000 MB)
= 3 851 063 DVDs (4.7 GB single layer)
= 4.6 km stacked DVDs = 462 km DVDs length in a row

Zoom video conferencing

Meeting hours
172 682
with
231 020
participants

Active Zoom users	509
Meetings	62 768
Webinars	24

Business travels

Staff travels

293

Business travels	190
Online events	103

Funded user travels
109

BeamStop

Sold meals
18 761

Sold Franzbrötchen
1927

Used fruits and vegetables
3752.5 kg

Consumed coffee

2127 litres

Protective COVID-19 measures

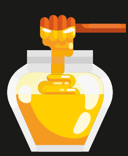
Surgery masks ordered	10 000	✓
FFP2 masks ordered	12 000	✓
Antigen test kits ordered	16 000	✓

Free apples and pears for staff
1.2 t = 1200 kg
= 6000 pieces

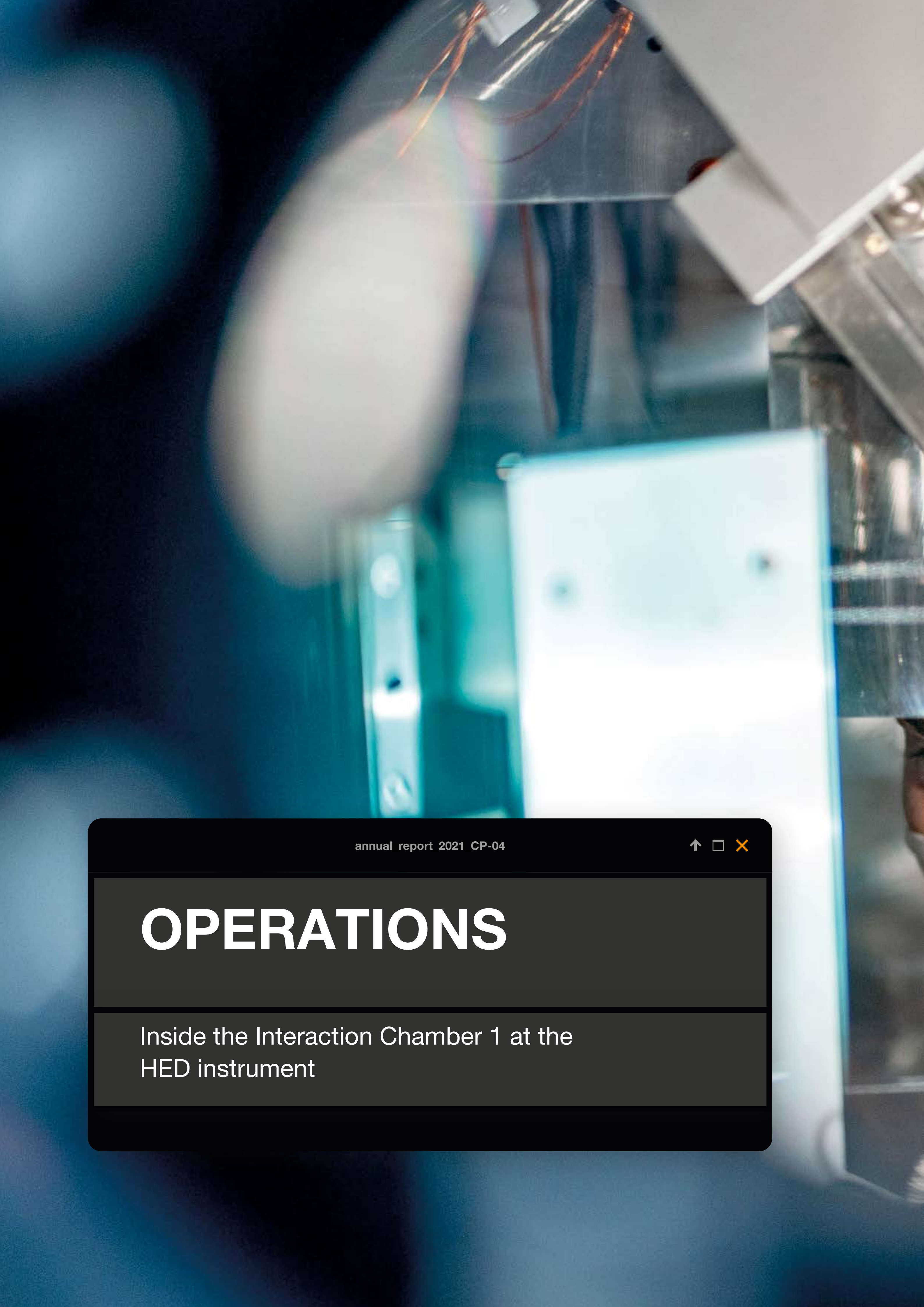
BEETIME 2021

Harvested honey on campus

30 kg



56 x 500 g jars
20 x 100 g jars



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OPERATIONS

Inside the Interaction Chamber 1 at the HED instrument

Operations

Although accelerator and user operations were still affected by the pandemic conditions in 2021, record performance was achieved in both areas. The most notable accomplishments were the excellent stability and availability of the accelerator, a new way to schedule the use of the X-ray beam, and the introduction of the Data Operation Centre.

Because of the COVID-19 pandemic, the need to reduce staff presence on site, and the difficulties for users to travel to Schenefeld, the European XFEL management decided to postpone the start of the user experiment programme. While X-ray delivery had originally been planned to begin at the end of February, the requirement to reduce onsite presence, in particular, led to a delay of one to two months. By the end of March, a prioritized science programme was started at the SPB/SFX instrument, targeting research related to the fight against the COVID-19 virus. The other scientific instruments received beam only by mid-April.

Due to the delayed start, only 9 of the 34 user experiments originally scheduled for the first half of 2021 could be allocated. To reduce the impact on the user programme,

fig-1_yearly-operation-hours_2021.xlsx

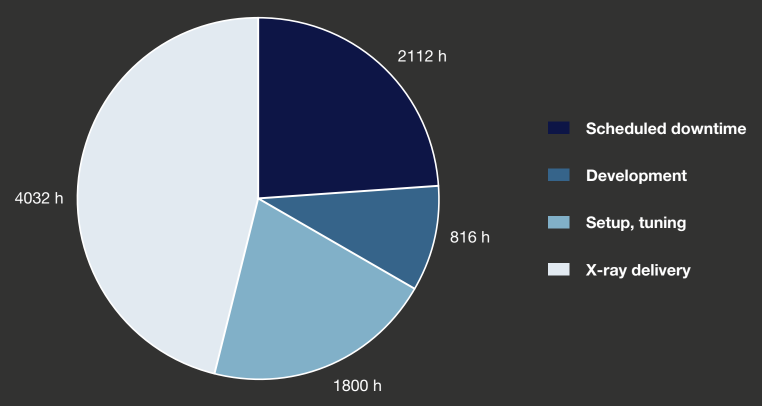


Figure 1:
Distribution of yearly operation hours of the European XFEL accelerator in four categories

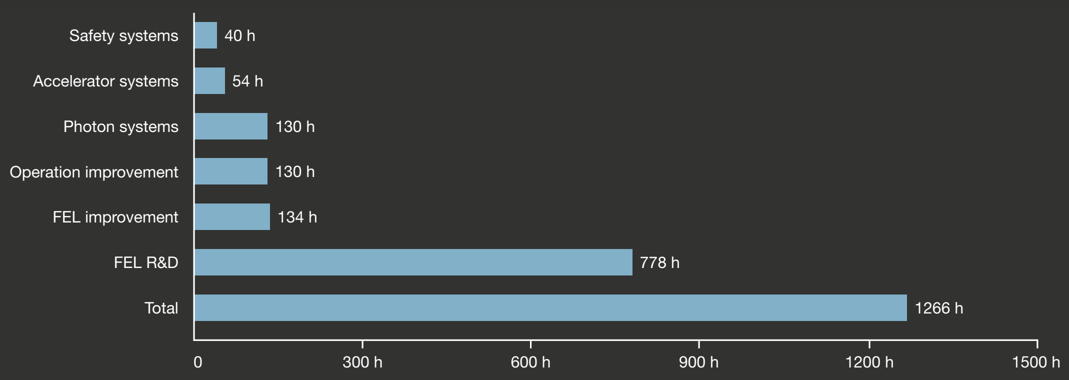


Figure 2:
The sum of the operation hours scheduled for various facility development activities exceeds the hours for development indicated in Figure 1, reflecting the parallel use of the facility for multiple activities.

the management decided that all experiments not receiving beam would either be shifted to the second semester of 2021 or to the first semester of 2022. After the summer maintenance period, a total of 35 user experiments and additional internal activities could be scheduled in an almost regular fashion. However, due to the still prevailing site and travel restrictions, the experiments were mainly performed without users on site—most users participated remotely, while European XFEL staff members and local collaborators took over the control of the measurements on site. Despite this setback, most experiments were successful, reaching extremely good results.

The European XFEL accelerator ran reliably and stably throughout the entire year 2021. The accelerator complex—consisting of the injector, the 17.5 GeV superconducting linear accelerator, and the electron beam distribution and beam transport systems through the three undulators to the beam dumps—was operated with beam for 6648 h (Figures 1 to 3). The handling of the complex superconducting accelerator and its subsystems has matured significantly, as was confirmed by the high uptime, excellent stability, and outstanding FEL performance observed (Figure 4). The delayed start of the X-ray delivery programme in spring was used to successfully boost the performance of the FEL delivery and continue the implementation of hard-X-ray self-seeding at the SASE2 FEL (see report on page 36).

Continuous improvement of the accelerator and FEL performance was achieved through both optimized operation and dedicated development. An outstanding accomplishment was the deployment of a longitudinal intra-train beam stabilization system in addition to the already operational transverse system, which allows the electron beam arrival time to be stabilized below 10 fs (RMS) both within a pulse train and over long time periods. The FEL performance was improved in terms of photon energy (reaching 24 keV at SASE1 and 30 keV at SASE2), pulse energy (yielding 17 mJ at SASE3), pulse length (approaching <10 fs at SASE2 and SASE3 using various bunch shaping techniques), and spectral brightness (by delivering hard X-ray self-seeding to users, resulting in an increase by up to a factor of 8 over standard SASE operation).

A special feature of the operation of the European XFEL accelerator is the ever varying X-ray delivery requirements, as specified by the experiments at the scientific instruments. To meet these requirements, the accelerator was operated at various electron energies between 11.5 and 16.3 GeV, with bunch charges of 100 and 250 pC, and using a plethora of electron bunch distribution patterns. In the past, this huge flexibility of the X-ray delivery and the varying requirements of the user experiments and internal activities had led to changes of the X-ray delivery conditions on a 12-hour basis to accommodate the different requirements of the two instruments located at each of the SASE FELs as well as during the week to meet the requirements of individual experiments. As a consequence, the delivery conditions were changed many times within a single week, often back and forth several times.

In early 2021, it was realized that this frequent switching led to a huge loss of time, as the accelerator, the FELs, and the X-ray delivery had to be tuned and the beam measured and re-adjusted after each change in delivery conditions. This also meant a huge workload on the instrument staff

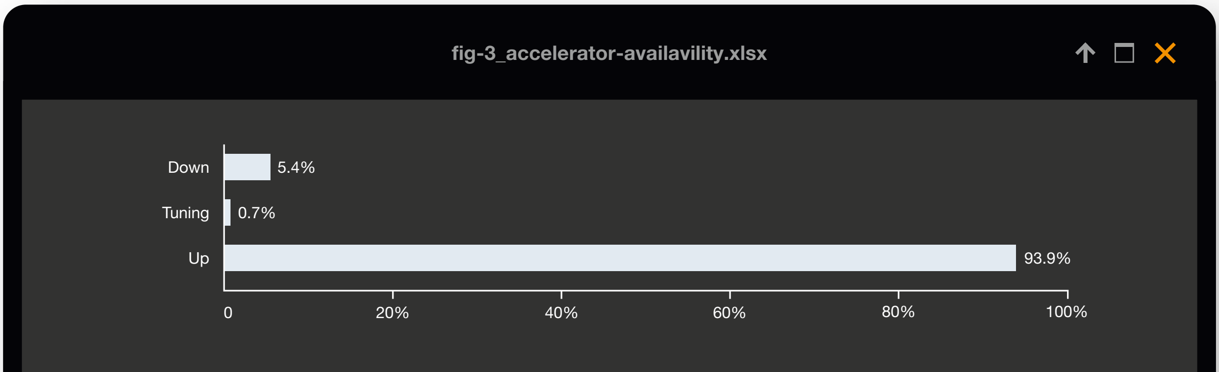


Figure 3:
Availability of the accelerator during FEL delivery mode in percent

fig-4_pulse-energy-statistics_2021.bmp

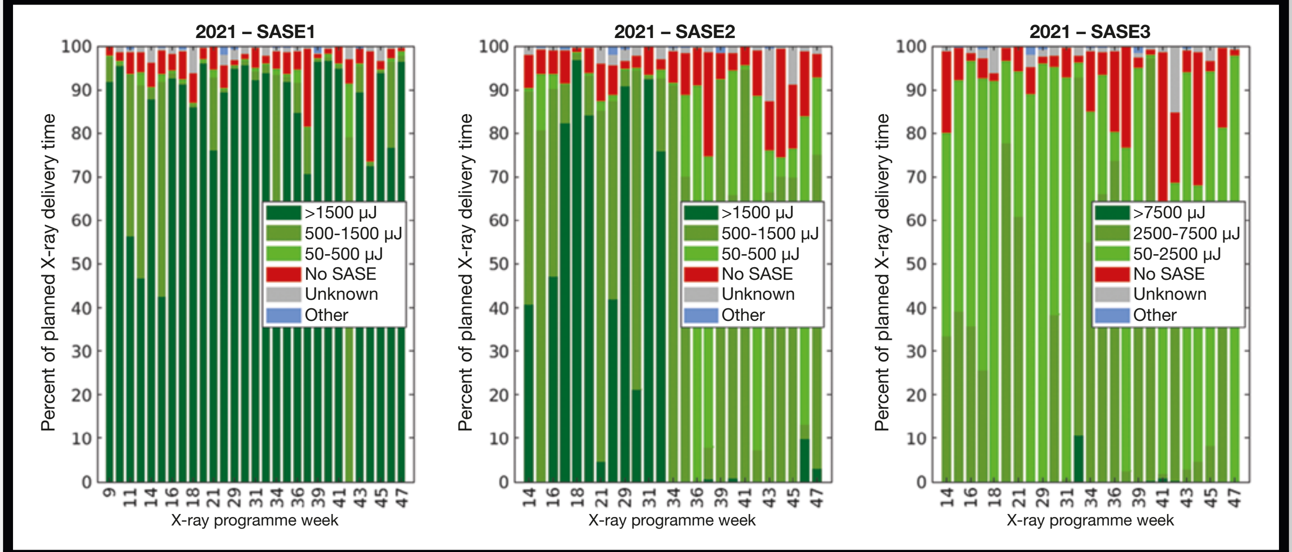


Figure 4:
Pulse energy statistics of the SASE1, SASE2, and SASE3 FELs achieved during X-ray delivery in 2021. The classification of the pulse energy performance depends on the FEL and the photon energy. While SASE1 was mostly operated for maximum pulse energy, many special delivery modes associated with smaller pulse energies were scheduled at SASE2 and SASE3.

and as well a limitation of the X-ray delivery and instrument performance. Now, operation is performed in the so-called priority mode, where one scientific instrument at each SASE FEL is given priority for a full week of scheduling. In the priority mode, the team at the priority instrument decides to either take beam for the full time or give part of the time to the other instrument at the same beamline. In case beam is given to the other instrument, the main delivery conditions (e.g. photon energy, beam pointing) should not be changed significantly in order to make the switching of the beam delivery minimally disturbing.

The priority mode also enables emphasis to be placed on experiment support during the period from 07:00 to 23:00 on all beam delivery days in a week. During this time, users and instrument staff receive a high level of support, while support is reduced during night-time hours. This support model assumes that the experiment teams schedule less demanding and complex activities at night, requiring less support from European XFEL staff members. It uses the European XFEL resources more efficiently but requires external user groups to perform their experiments continuously over several days.

One of the 2021 activities to improve support of the experiments was the establishment of the Data Operation Centre (DOC; see report on page 39). Since the start of X-ray delivery in March, the DOC has played a very important role in making operation smoother and more successful.

Scheduling using the priority mode started in April for a test period. The achievements of the priority mode and the new support models were analysed first in summer and then in late 2021. The operation was much smoother, less time was lost for beam switching, and experiment success was increased. No major issues related to the reduced support were found. The priority mode was thus confirmed as the standard mode of scheduling instrument activities in 2022.

Out of the total operation hours of the accelerator, X-ray delivery to the experiment hutches was scheduled for 4032 h, and the availability, measured as the fraction of time in which SASE photons are actually generated within the scheduled period, was about 94% averaged over all three FELs. This excellent number resulted from the diligent and creative work of all of the people involved in the operation, both at DESY and at European XFEL. Parallel allocation of user experiments and internal activities at the three FEL sources led to an overall scheduling of 8264 h of X-ray delivery at the six scientific instruments.

fig-5_2021-User-experiments.xlsx

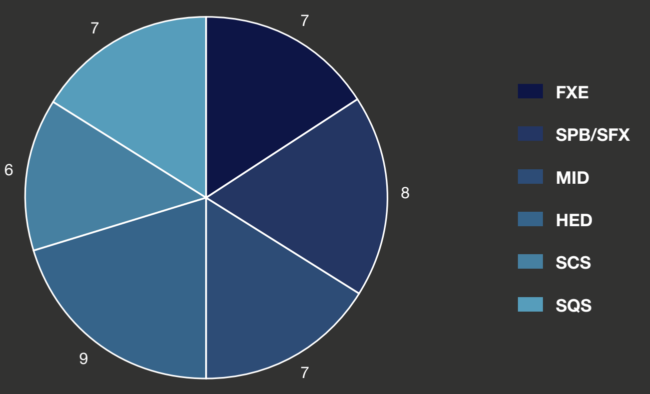


Figure 5:
Number of user experiments allocated beamtime at the six scientific instruments in 2021

While accelerator and FEL availability has been extremely high, for the individual scientific instruments and the user experiments, it is important that the X-ray beams are delivered to the sample within a required performance window. This area still experiences problems, mostly related to frequent beam position instabilities, in particular after the SASE1 and SASE2 X-ray beam transport systems. During the year and the winter maintenance period, many investigations were conducted to identify the root causes of slow and fast beam movements as observed at the end of the delivery tunnels or at the sample positions of the scientific instruments. Several new diagnostic devices have been installed and are being commissioned, and new measurement protocols and monitoring tools have been established. Through close collaboration of the scientific instrument groups and the Development and Operations groups, the response time following the observation and reporting of beam instabilities has been greatly reduced. The plan for 2022 is to enforce the monitoring of beam position instabilities and to correlate these with measurements of environmental parameters in order to better identify root causes and to develop mitigation scenarios based on this knowledge.

Another issue in the X-ray beam delivery to the scientific instruments is dependencies of the beam properties, due to crosstalk, on changing conditions at the other FELs. The European XFEL is operated with highly complex beam delivery patterns prepared by the electron accelerator, while individual experiments have the possibility to change some of these parameters (photon energy, number of X-ray pulses per burst, pulse pattern) as needed. While feedback mechanisms for the electron beam delivery handle these changes better and better, these effects are observed in particular at the two successive FELs, SASE1 and SASE3, and at the instruments located there.

In 2021, most of the operational safety limits that had been introduced to avoid the risk of damaging radiation protection units, such as beam shutters and beam stops, were lifted. In a joint effort of DESY and European XFEL groups, the potential of the (focused) X-ray beam to burn through various materials used for these devices was clarified in several measurement campaigns. Based on the results of these measurements, a concept for redundant beam stoppers and monitors was developed and implemented in the beam transports and scientific instruments. In particular, active instrument beam stops, now installed in each of the instrument hutches, made it possible to lift the operational safety limits, thus enabling the scientific instruments to benefit from the full X-ray flux offered by the accelerator and the FELs.

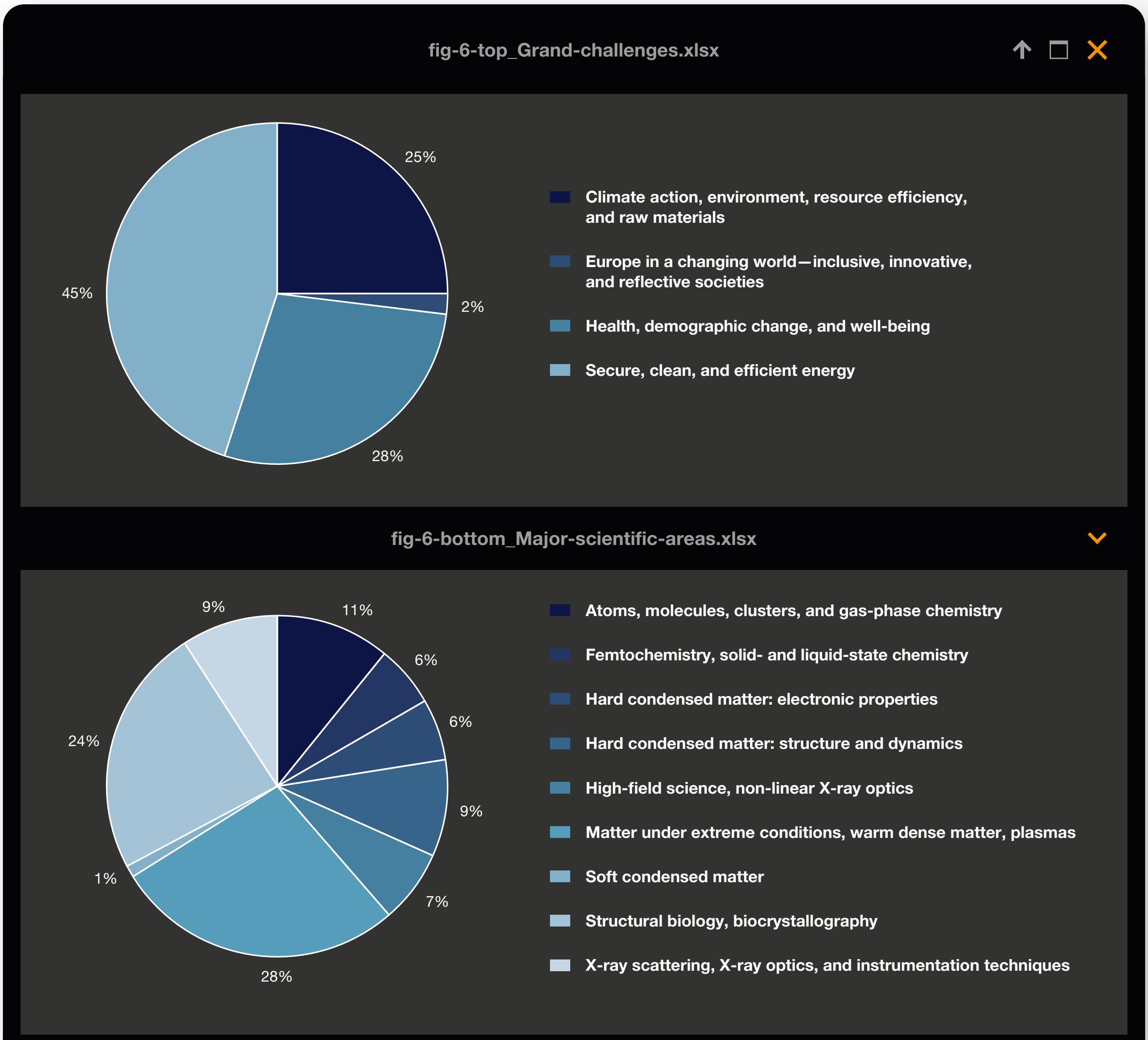


Figure 6:
Distribution of users according to grand challenges (top) and major scientific areas (bottom)

The infrastructure required to support the operation—the cryogenic plant as well as the power, water cooling, air conditioning, IT infrastructure, and safety systems—has essentially been in operation 365 days per year. A notable achievement in 2021 was the further reduction of vulnerability to brief voltage variations in the main grid, resulting in less interruption of the European XFEL operation during the summer months compared to user facilities on the DESY campus. Towards the end of 2021, changes in the infrastructure were also made on the Schenefeld campus to reduce this dependency on voltage variations in the main grid here too.

The 2021 user programme included the allocation of 44 proposals, which received a total of 4664 h of X-ray delivery time. These 44 experiments were related to a total of 1004 user visits, both on site and remote. Only a small fraction of the users were present on site, while a majority participated in the experiments remotely. The 1004 user visits corresponded to 702 individual users, of which 220 were present on site. Figures 5 to 7 show the distribution of user experiments at the six scientific instruments, the assignment of user experiments to the grand challenges and major scientific areas, as well as the distribution of individual users according to their countries of affiliation.

Only one new call for proposals was initiated in 2021, due to the decision to re-allocate user experiments that could not be performed in 2021 to the first half of 2022, making a new call for that allocation period unnecessary. The 8th call for proposals for experiments during the second half of 2022 had a deadline in November 2021 and yielded 167 proposals.

fig-7_user-distribution_by-country_2021.xlsx

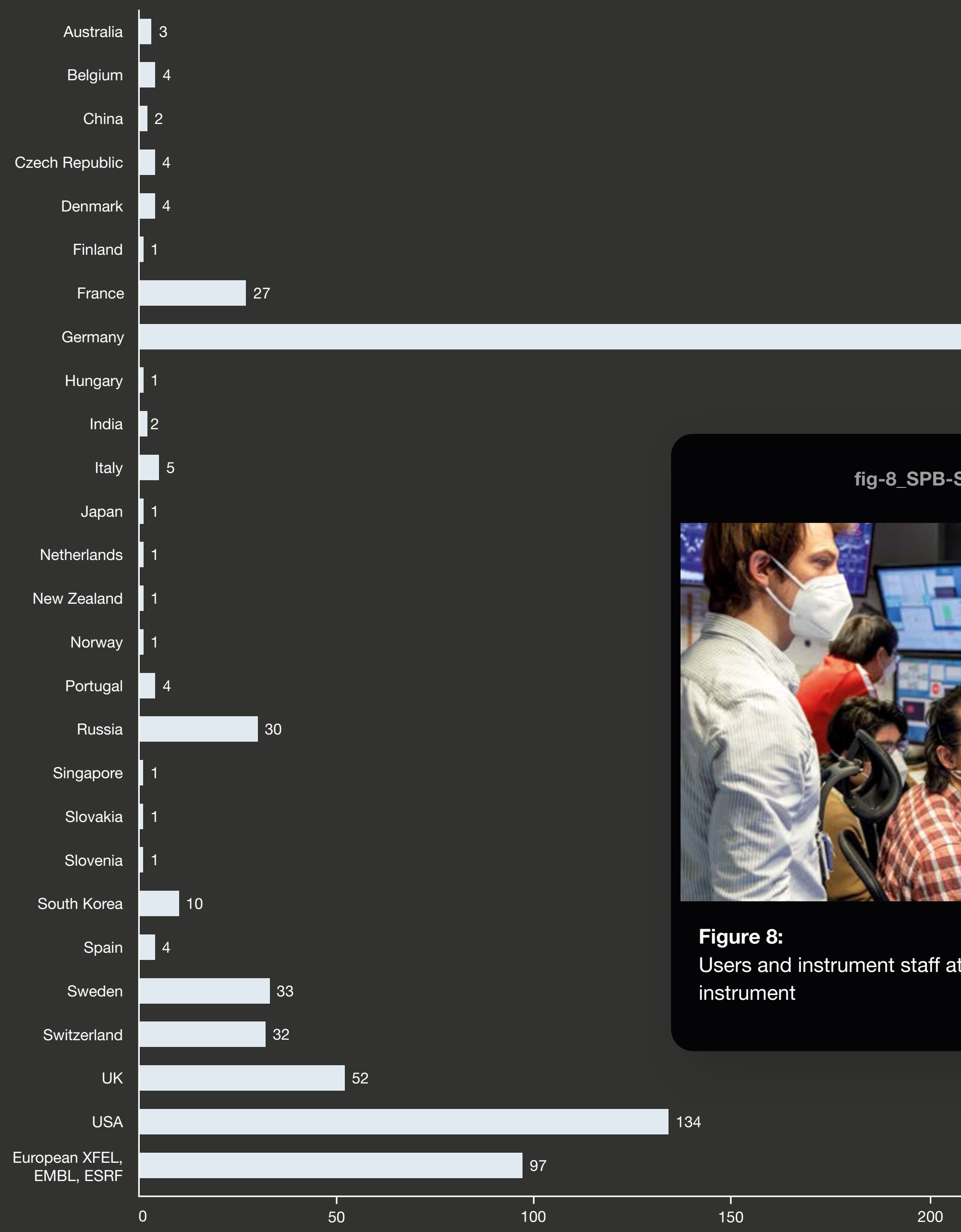


Figure 7:
Distribution of individual users participating (mostly remotely) in experiments in 2021, shown by country of affiliation

fig-8_SPB-SFX_users.jpeg

Figure 8:
Users and instrument staff at the SPB/SFX scientific instrument

An Experiment Hall Crew (XHCrew) Coordinator was hired as the first member of a new team supporting the operation of the experiment hall and the experiments performed there. Regular presence of an XHCrew member on shift is expected to start in 2022. Safe operation of and within the experiment hall has been a focus of the new XHCrew Coordinator, something that has already led to the reduction of fire load, the proper posting of standard operation procedures on parked components, and the implementation of storage concepts. The X-Ray Operations (XO) group got more involved in the process of scheduling user experiments and internal activities in 2021 with the aim to simplify it. The schedule for the first half of 2022 is a first result of this effort, and XO seeks to continuously improve this process.

FACILITY UPDATE

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

Campus Development

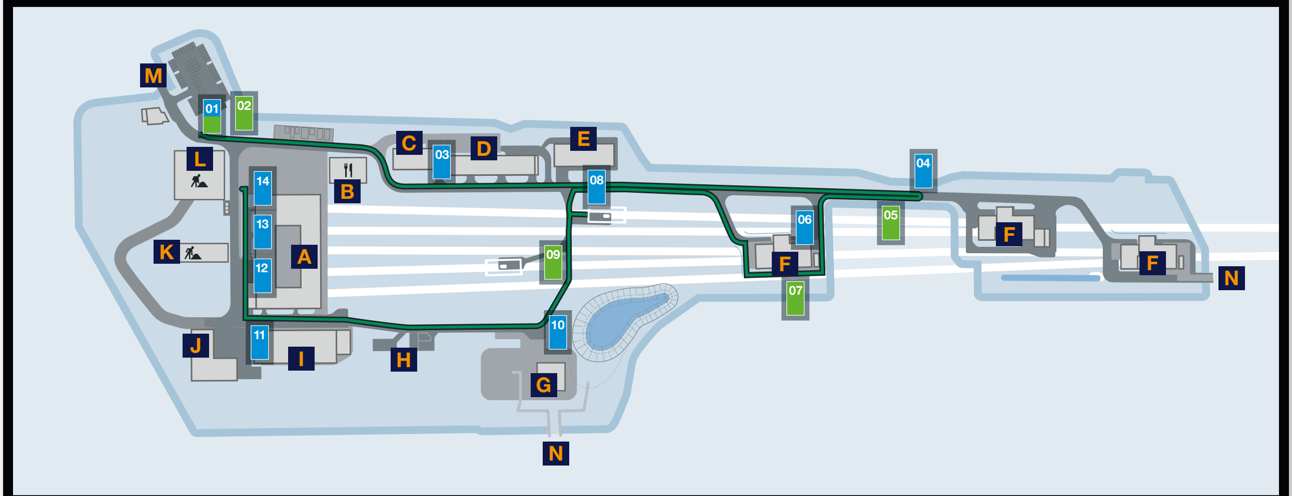
In 2021, the new guest house and the undulator hall were taken into operation, the campus infrastructure was perfected, and big steps were achieved for the new office building and the visitor centre.

While the European XFEL campus in Schenefeld was fairly deserted for a good part of 2021 due to pandemic-related access restrictions, many elements of the still very new campus were completed and put into operation. These tasks were mainly coordinated and supervised by the Technical Services group, working together with many groups at European XFEL and DESY as well as external companies.

The guest house was inaugurated in June and welcomed first users in the same month. The undulator hall was handed over to the Undulator Systems group in January and immediately put into operation. The handover of the commissioned measurement rooms took place in September. The technical gas storage and dangerous materials storage areas were also put into operation in June. With the completion of the guest house, the third entrance to the Schenefeld campus was opened in May.

The Communications group devised a campus info tour (Figures 1 and 2), which was implemented during the year. The tour is intended as information for visitors entering the campus and as an opportunity for our staff members and guests to learn even more about the facility. Fourteen panels provide information about the underground facility and buildings, their function, and the activities that take place within them (blue panels) as well as information about environmental compensation measures and the natural landscape on the campus (green panels). The info panels are connected by a green line painted on the ground, which forms the 1600 m long info tour.

fig-1_schenefeld-campus-plan-AR21.ai



- **A** Headquarters/experiment hall (XHQ/XHEXP1)
- **B** BeamStop restaurant and cafeteria
- **C** Central electrical station (XHPSC)
- **D** Pump station and cooling (XHPSC)
- **E** Undulator hall (XHU)
- **F** Tunnel entrance buildings (XHE2–4)
- **G** Guest house (XHG)
- **H** Dangerous materials store (XDMS) and technical gas storage (XTGS)
- **I** Ventilation and air conditioning (XHVAC)
- **J** Central workshop and storage (XHWS)
- **K** Office building (XHO)
- **L** Visitor and conference centre, school labs (XHV)
- **M** Main entrance and gate house (XHGATE)
- **N** Side entrances

fig-1_note.txt

Figure 1:
Schenefeld campus plan with the campus info tour (green line) and the new info panels (blue and green numbers)

Figure 2:
Installation of the info tour panels in February 2021

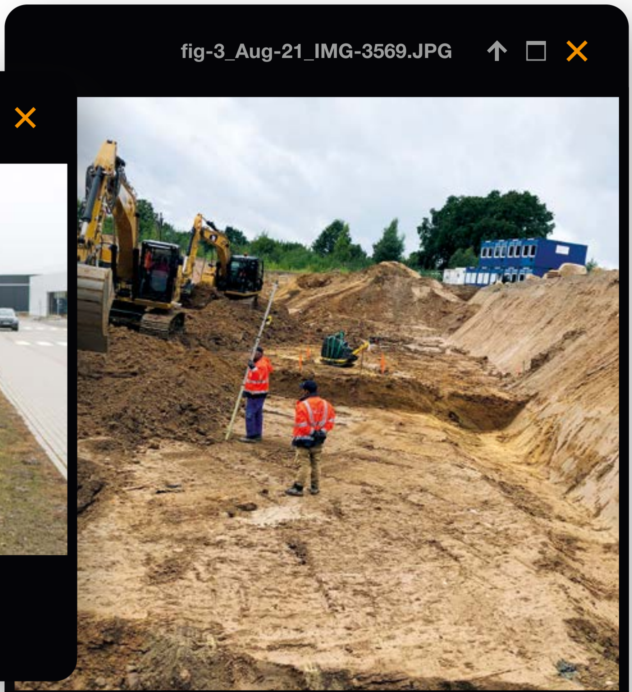


Figure 3:
Groundbreaking for the new office building in August 2021

The campus not only improved on the outside, there were numerous construction and improvement activities inside the buildings as well—in particular in the experiment hall, where the construction work for a third scientific instrument at the SASE3 FEL source was completed. These activities included the modification of the existing hutch structure and the creation of two new rack rooms and one control room. Together with the newly formed experiment hall crew, the operation and storage concept for the hall was revisited, and space was made for a new control room for this team, facilitating operations in the experiment hall from summer 2022 onward.

An important activity was to make the facility and its subsystems more resilient to fluctuations in the power supply: After a major power outage in August, the cooling water pumps of the laboratory floor in the headquarters building were switched to an uninterruptible power supply, and a flap was reprogrammed to separate the cooling water networks of the pump station and cooling building from those of the headquarters building until both systems are back in operation after power outages. These two measures have led to a significant stabilization of the cooling water circuits, especially following short power outages, and thus of the systems that require an uninterrupted cooling water service. In addition, many more refurbishments and improvements of the air conditioning, cooling water treatment, technical gas supply, and compressed air supply systems were completed.

Buildings and facilities in Schenefeld were further developed and improved, with the goal of facilitating work and enhancing experience for our staff members, users, and visitors. Major milestones were achieved in 2021, e.g. the groundbreaking for the new office building in August (Figure 3). At the end of the year, the construction work progressed according to plan. The goal is to have the building operational in early 2023 and then demolish the temporary offices, where many staff members have had offices since 2015, when first activities started on the Schenefeld campus.

Important administrative and planning milestones were reached for the new visitor centre, which are necessary to start civil construction in 2022. By the end of the year, European XFEL submitted the legal documents required for the tendering of the construction works. The development of the interior design of the visitor centre and the school labs made good progress. The planning of the exhibition, the cinema, and the virtual-reality rooms in the visitor centre was completed, and the tendering process for the realization of the exposition was started.

Facility Development

While the focus of daily activities at the European XFEL shifts more and more to performing experiments, a multitude of development activities are either continuing or starting. These activities include mechanical, software, and procedural work in all areas of the facility and will further improve performance to keep our leadership in the field of high-repetition-rate X-ray FELs.

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

Apart from regular X-ray photon delivery, yielding record FEL photon energies and intensities, important developments have been made to the accelerator and the FEL sources. The operation year 2021 included two maintenance periods totalling about six working weeks. For the accelerator systems, this time was required to perform standard preventive maintenance, repair installed components, and make new installations. The largest new installation in 2021 was the addition of four APPLE-X–type undulators to the SASE3 FEL. The undulator design was developed by the Paul Scherrer Institute (PSI) in Switzerland and adapted to the European XFEL requirements in terms of magnetic period, gap, and space limitations. APPLE-X undulators offer a wide range of possible polarization modes and magnetic gaps, which were carefully measured and optimized by the Undulator Systems (UNSYS) group. These additional undulators will operate in tandem with the planar undulator segments of SASE3 in the so-called afterburner scheme and provide nearly arbitrarily polarized FEL radiation for soft X-ray user experiments at the SASE3 scientific instruments.

For this major addition to SASE3, preparations of the electron beam transport section started as early as 2020. After an intense period of preparing new beam vacuum chambers and undulator segments, installation took place in the 2021–2022 winter maintenance period, including removing the old vacuum system, moving in the new undulator segments, reconnecting the new vacuum system, re-establishing vacuum conditions, and completing the electronic cabling of the new segments. The transport of the four bulky 8 t segments on air cushions from the XS4 shaft to their final position in the electron beam transport was a particular challenge (Figure 1). By the end of the winter maintenance period in January 2022, the mechanical and electrical installation was successfully completed and the undulator segments were ready for commissioning (Figure 2).

fig-1_APPLE-X_transport.JPG

Figure 1:
Transport of one of the APPLE-X undulators into the European XFEL undulator tunnel

fig-2_APPLE-X_segments.JPG

Figure 2:
Four new APPLE-X undulator segments installed at the end of the SASE3 undulator

Behind the SASE2 undulator, a so-called corrugated structure was installed in the accelerator vacuum system. This structure consists of a 5 m long narrow vacuum chamber in which the electron bunches create wakefields that act back on the very bunch and create an energy variation along it. A screen downstream of the device makes it possible to observe the energy variation and to establish a measurement that is sensitive to the longitudinal position along the bunch—similar to transverse streaking but using a passive structure. The device provides insight into the lasing process, in particular which part of the electron bunch participates in the lasing. Commissioning is scheduled for early 2022.

Finally, in the electron dumps areas, the vacuum pumps were relocated. In their previous location, a high radiation background had led to instability and a shortening of their lifetimes.

In order to improve the online measurement of the spectral properties of the X-ray beams, the X-Ray Photon Diagnostics (XPD) group developed an angle-resolved hard X-ray photoelectron spectrometer (hxPES) dedicated to non-invasive and pulse-resolved photon diagnostics at the SASE1 beamline. Prior to installation, the device was successfully tested at the DESY PETRA III synchrotron (Figure 3). Record-breaking retardation voltages of more than 8 kV were achieved, allowing spectral beam monitoring over a wide range of hard X-ray photon energies. The hxPES device was installed in the SASE1 beamline during the 2021–2022 winter maintenance period and will be tested with the X-ray beam in 2022.

In a second project, pulse-resolved images of the beam pattern from arbitrary pulses within an X-ray pulse train were acquired. A high-speed camera (Shimadzu HPV-X2) was connected to one of the X-ray beam imagers in the tunnel, making it possible to record 128 images at up to 4.5 MHz repetition rate within a pulse train. The results of the measurements were used to study beam position stability. It was possible to correlate the electron beam orbit with the transverse X-ray beam position in a pulse-resolved fashion. The measurements will make it possible to enhance beam stability along the X-ray pulse trains.

fig-3_DESY-PETRA-III-synchrotron.pdf

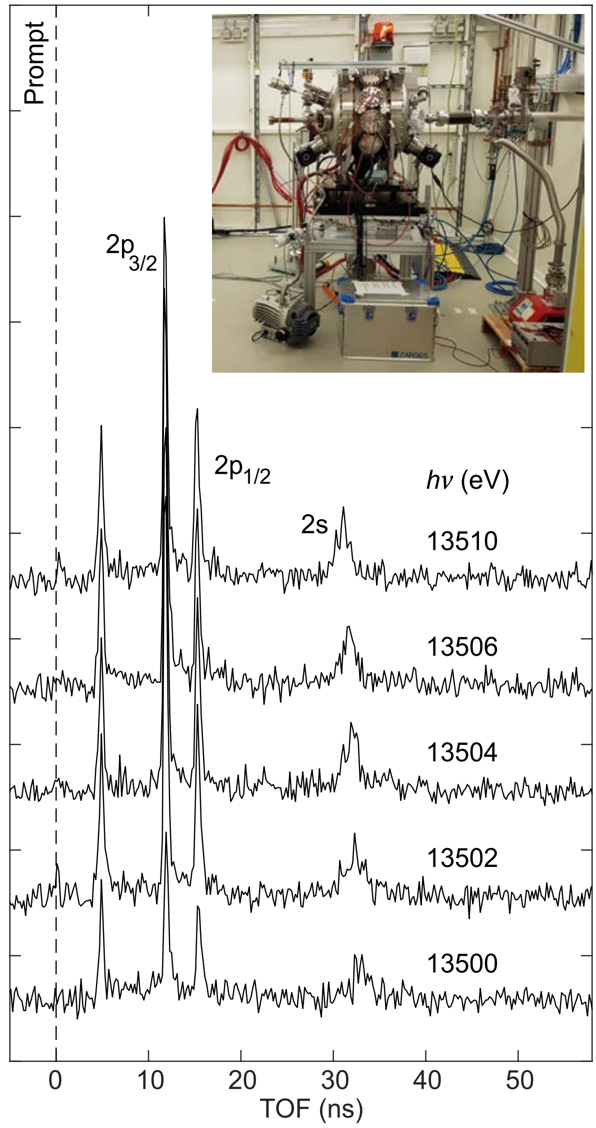


Figure 3:
Time-of-flight (TOF) spectra, recorded with the new angle-resolved hxPES device, showing the X-ray photon energy near 13 keV. Data were taken at the P09 beamline of the DESY PETRA III synchrotron using xenon gas and a photoelectron energy retardation of 8 kV. The insert shows the experiment setup.

The SCS instrument and X-Ray Optics (XRO) groups successfully upgraded the soft X-ray monochromator at SASE3 to higher energy resolution. The monochromator was equipped with a short 50 lines/mm grating, providing resolving powers of around 3000, suitable for a wide range of X-ray spectroscopy applications. With the installation of the high-resolution Heisenberg resonant inelastic X-ray scattering (hRIXS) spectrometer at SCS, allowing users to study the evolution of low-energy excitations in complex materials with unprecedented time and energy resolution, the resolving powers of the monochromator and the spectrometer had to be matched. A new grating for the monochromator of same length as the existing one, but with a higher line density (150 lines/mm), was specified at the beginning of 2020. Due to the large distance of 100 m from the grating to the exit slit, very tight demands on the varied-line spacing (VLS) parameters challenged the production of the grating by the commercial supplier. The grating was finally delivered at the end of 2020 within the specified tolerances, coated with B4C, characterized in the XRO metrology laboratory, and installed during the 2020–2021 winter fig-4_SASE3-high-res-grating.JPG

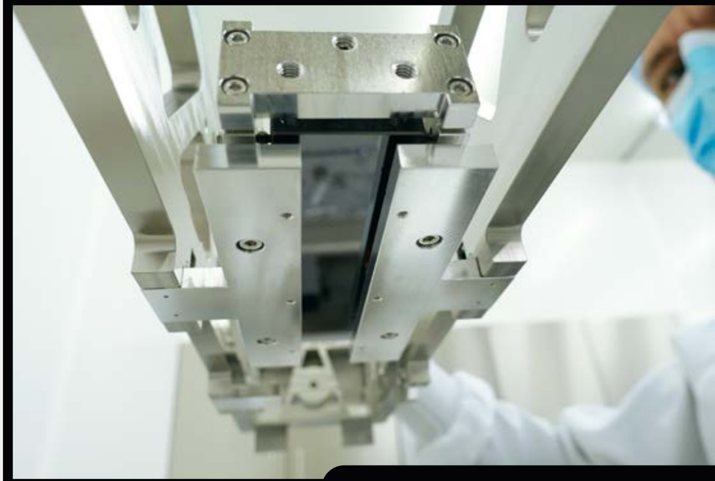


fig-4_note.txt

Figure 4:
Photograph taken upwards looking at the face of the new high-resolution grating for the SASE3 soft X-ray monochromator, installed on the mirror mount in the metrology laboratory

fig-5_XFEL-raw-data.eps

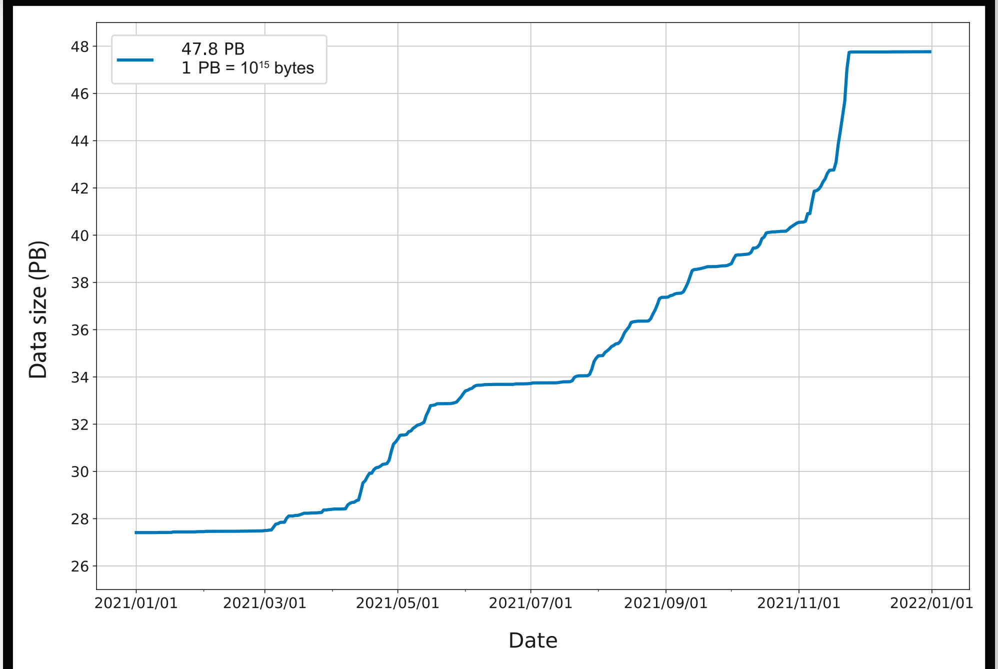


Figure 5:
Time evolution of the raw data generated at the European XFEL scientific instruments in 2021

maintenance period by the XRO and Vacuum (VAC) groups (Figure 4). The grating was commissioned, together with the hRIXS spectrometer, in April–May 2021 by the SCS group together with members of the hRIXS User Consortium. The targeted resolving power of 10 000 was confirmed for the energy range between 500 and 1000 eV, i.e. at the oxygen K- and copper L-edges. Since summer 2021, the high-resolution upgrade of the monochromator has been available to all users of the SASE3 soft X-ray monochromator. In addition, it enhances the spectral resolution of X-ray diagnostic tools in SASE3.

Detectors and data science

In 2021, the maturity of data systems and of the infrastructure needed to operate the scientific instruments was continuously improved. This was clearly demonstrated by the increase in integrated raw data generated over the course of the year, culminating in November in a sustained two-week period in which 5 PB of raw data were acquired (Figure 5). When the data produced by the calibration of the raw data is considered, over 7 PB of data were created, stored, and catalogued in the last seven days of the run.

Such data throughput clearly illustrates that the acquisition, storage, and computing infrastructure, together with the processing pipelines and the algorithms that form the overall data-taking architecture, were developed and optimized to a point at which the very large data rates produced by a MHz X-ray FEL using 2D Mpx imaging detectors can be handled and lead to scientific results. Further consideration showed that, while the MHz rate of the accelerator and detectors drive the peak data rates, it is the sustained and efficient operation of the scientific instruments over the course of several parallel experiments that determines the overall amount of data taken.

Sustained and efficient operation is enabled by the underlying infrastructure, which was successfully commissioned over the last years, is constantly maintained, and continues to be further developed. Highlights in 2021 have been the optimization of the detector calibration pipelines, which achieved sustained processing of a complete DSSC detector train within the 10 Hz readout cycle, the conception and commissioning of the Data Operation Centre (DOC), which builds on the technical capabilities provided by the introduction of the Grafana monitoring tool coupled to an InfluxDB time series database, and finally the continued improvement of the programmable logic controller (PLC) infrastructure and cabling, which included over 450 PLC modules modified and more than 14 km of cables installed.

With this level of data now regularly being taken, even during COVID-19–affected operation, the European XFEL data reduction and retention policies and procedures that were put in place in 2017 at the start of operation will have to be reviewed, adapted, and strengthened using input from the research done over the past two years.

Scientific instruments

A major activity in 2021 was to improve the timing capabilities for pump–probe experiments using the optical laser. Activities involved the scientific instrument groups, the XPD group, the Optical Lasers (LAS) group, as well as the MSK LbSync group at DESY, which is responsible for laser-based optical synchronization systems. The FXE and SPB/SFX instrument groups made significant progress in the implementation of the pulse arrival time monitors (PAMs) at their instruments, supported in particular by the XPD group for the PAMs and by the Data Department groups for the integration.

For FXE, it is crucial to precisely monitor the time delay between the optical femtosecond pump pulses and the X-ray probe pulses, which changes from shot to shot, mainly due to different time references for the electron and optical laser beams. The measurement of the relative arrival time of both pulses is important for subsequent sorting and binning of the experiment data and might also serve to select signal regions of interest in the temporal domain. A simple, robust, and user-friendly PAM, designed by the XPD group (Figure 6 left), was installed in the FXE X-ray hutch in 2021 and later commissioned with support from the XPD, Electronic and Electrical Engineering (EEE), and Controls (CTRL) groups. The PAM uses the spectral encoding technique, in which temporally stretched and chirped optical laser pulses and the X-ray pulses are overlapped in space and time on a 50 µm thick Ce:YAG target. The X-ray beam modifies the transmission of the YAG for the optical laser beam, thereby leading to a modification of the transmitted spectrum. A GOTTHARD-I detector, operating at 564 kHz, was used to record the optical laser pulse spectra for a reference pulse (564 kHz) and the X-ray

fig-6_FXE-PAM_PP-laser-timing.png

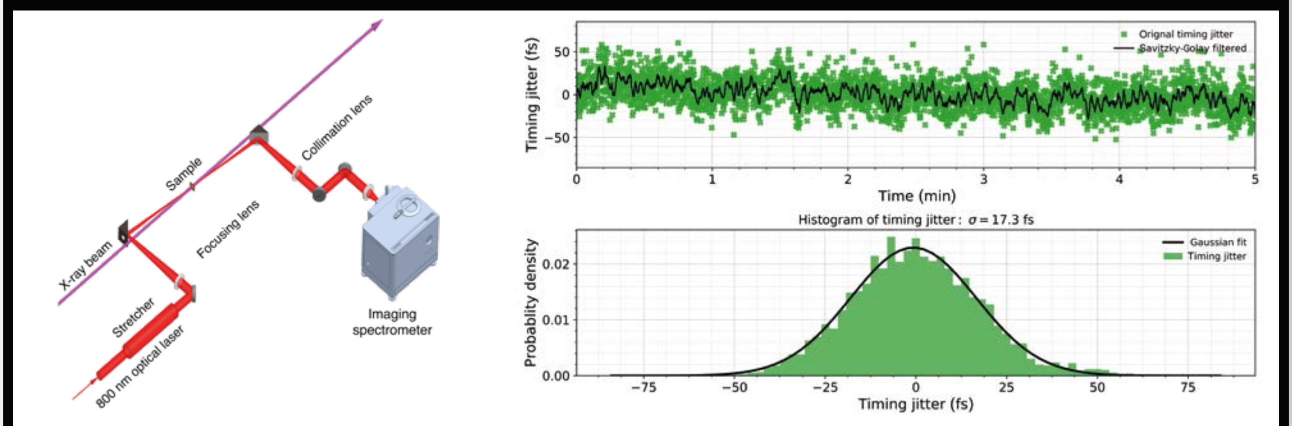


Figure 6:
Left: Rendering of the new FXE PAM. Right: Measurement of the timing jitter between the PP laser and the X-ray pulses as a function of time and jitter distribution.

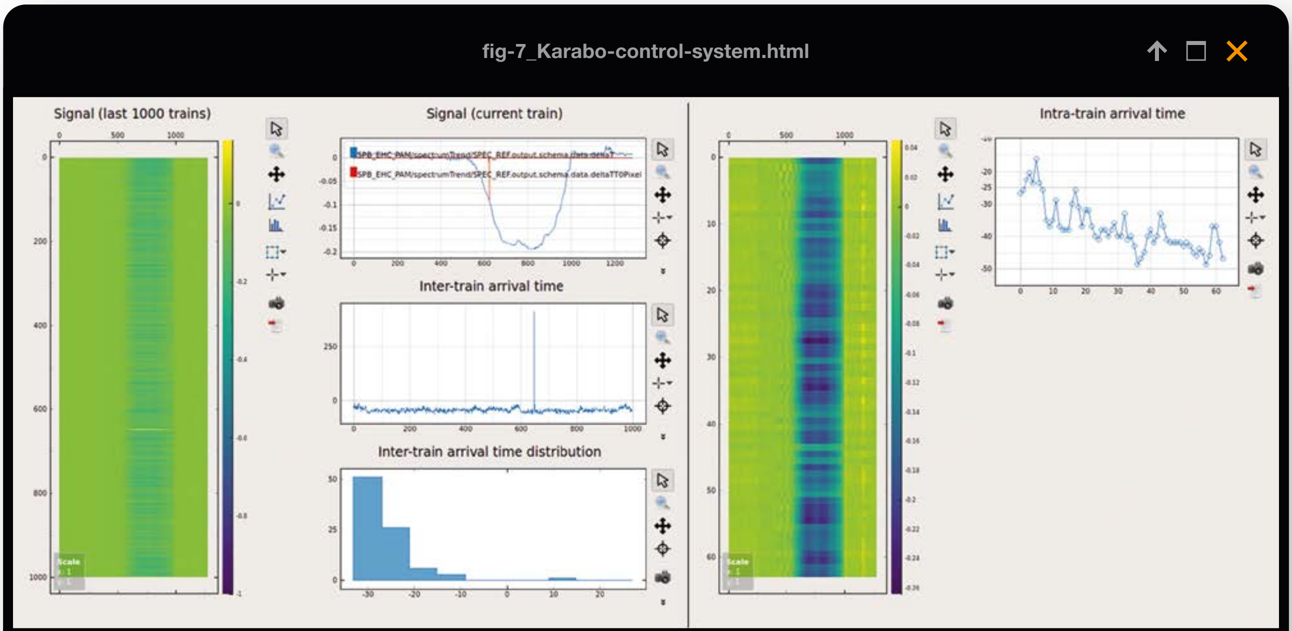


Figure 7:
PAM online analysis at the SPB/SFX instrument implemented in the Karabo control system

signal (282 kHz). Using optical synchronization of the SASE1 pump–probe (PP) laser, the timing jitter was measured at 17.6 fs (RMS), and no significant time zero shift was observed during the 5 min measurement (Figure 6 right). For FXE, the availability and functionality of the PAM is a first step towards higher time resolution. The optimization of the PAM signals and their integration will be an ongoing project in 2022.

At the SPB/SFX instrument, the PAM had already been installed and commissioned. In 2021, the instrument group and the Data Analysis (DA) group, in a joint effort, developed and implemented a high-performance online data analysis tool for this diagnostic device (Figure 7). The ability to analyse the PAM data online provides benefits to users and enables further improvement of the time arrival stability of the optical laser and X-ray pulses. For example, it was possible to directly observe the effect of electron beam conditioning on the arrival time of the X-ray pulses. This information can be used to optimize the operation of the accelerator for the best possible performance at the instrument where optical pump – X-ray probe experiments are conducted. In a collaboration of SPB/SFX, XPD, and DESY groups, excellent correlation between X-ray (PAM) and electron (bunch arrival time monitors, BAMs) diag-nostics could be demonstrated (Figure 8), thanks in part to these developments. The results of the PAM online data analysis are now integrated into the data provided to users, who may then use the information in further data-processing steps to improve the temporal resolution of their experiments.

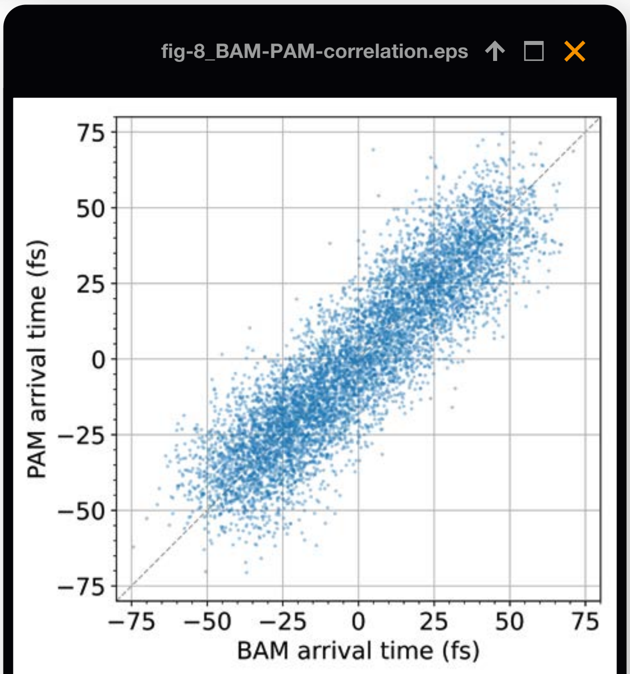


Figure 8:
Correlation between the arrival time of electron bunches relative to the reference optical clock (BAM), upstream of the SASE1 undulator, and between X-ray and optical laser pulses (PAM), at the SPB/SFX instrument

At the HED instrument, the ReLaX high-intensity optical laser provided by the HiBEF User Consortium was, for the first time, employed in a user community–assisted commissioning experiment to study the impact of the relativistic plasma environment on X-ray diagnostics. The objective of the user experiment was to validate the feasibility of small-angle X-ray scattering (SAXS), X-ray phase contrast imaging (PCI), and X-ray spectroscopy on a variety of targets covering multiple science cases, such as hole boring, relativistic transparency, fast electron transport along extended targets, isochoric heating of buried targets, equation of state (EOS) determination by shocked targets, as well as plasma instabilities in a relativistic intensity regime (Figure 9). In a cooperation between the HED and LAS groups and the HiBEF User Consortium, approximately 180 shots from the ReLaX laser were performed within three shifts on a variety of samples probed by the X-ray FEL beam. Overall, the objectives of the experiment were met and high-impact publications are expected as a result. Some of the commissioning results already triggered further developments of the used methods.

A second activity at HED was to employ the AGIPD mini-half prototype detector, installed and commissioned in 2020 in collaboration with the Detector (DET) group and the DESY Photon Science Detector Systems (FS-DS) group, for three user experiments proposed by international teams, performing MHz-rate diffraction experiments in diamond anvil cells in Interaction Chamber 2 (IC2), which was provided by the HiBEF User Consortium. All three experiments relied on the combination of the unique time structure (several X-ray pulses within a few-100 µs pulse train) and high photon energies, which are currently available only at the European XFEL. The use of the AGIPD detector was paramount to obtain pulse-resolved data within the train.

Organizing development activities

The development and implementation of new instrumentation and capabilities occur in parallel to the operation of the facility, which comprises the experiment programme and all the maintenance and continued support of the various subsystems of the European XFEL. To manage the new developments, the Project Management Office supports the establishment and execution of so-called development projects (DPs). The majority of DPs are requested by the scientific instrument groups in order to further develop the instruments, and resources are requested from the expert groups in the Development and Operations Division. A DP workflow defines the setup, structure, and approval of the projects and also allows for controlling and closing them.

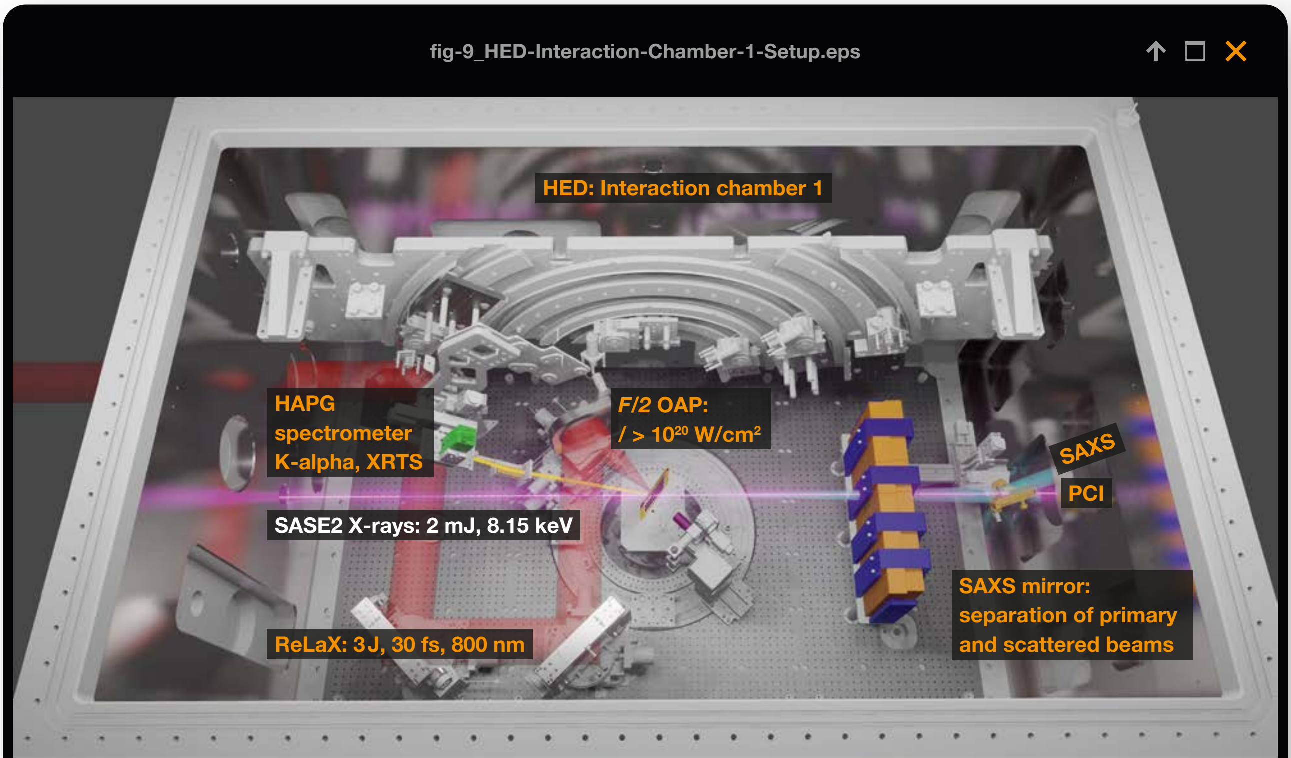


Figure 9:
Setup at the HED Interaction Chamber 1 combining the ReLaX high-intensity laser with SAXS, PCI, and X-ray spectroscopy

At the beginning of 2021, 16 projects approved in 2019 and 2020 were in progress. During the year, 6 of these projects were successfully closed and 13 new ones were approved. Another 7 new DPs were initiated in 2021 and are currently reviewed for approval (Figure 10). The overall budget of the projects approved in 2021 is close to 6 million euro (M€), half of which is associated with setting up a test facility for a new superconducting undulator DP pursued by the UNSYS group in collaboration with DESY.

The average budget of the remaining DPs is about 230 thousand euro (k€). The initiation of each DP involves estimating the work effort requested from the various expert groups (Figure 11). In general, the major part of the effort is requested from the groups in the Data Department, in particular from EEE due the general requirement for planning, procurement, and installation of PLC electronics and the corresponding cabling.

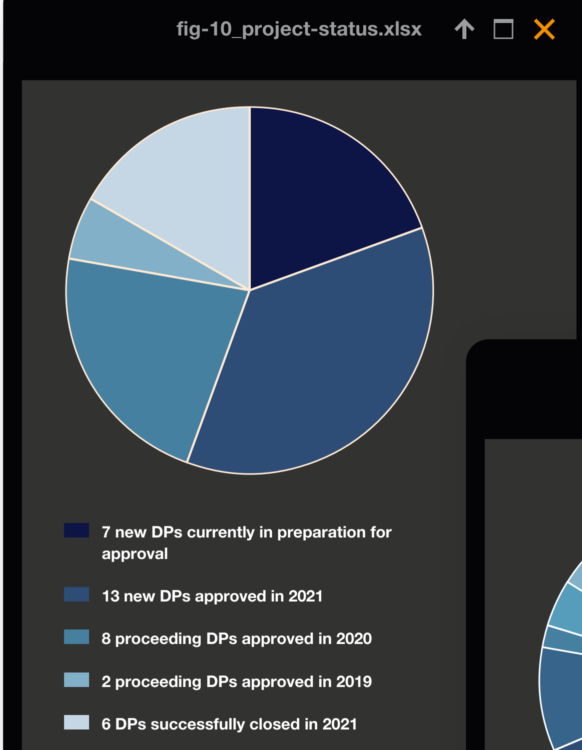


Figure 10:
Status of development projects

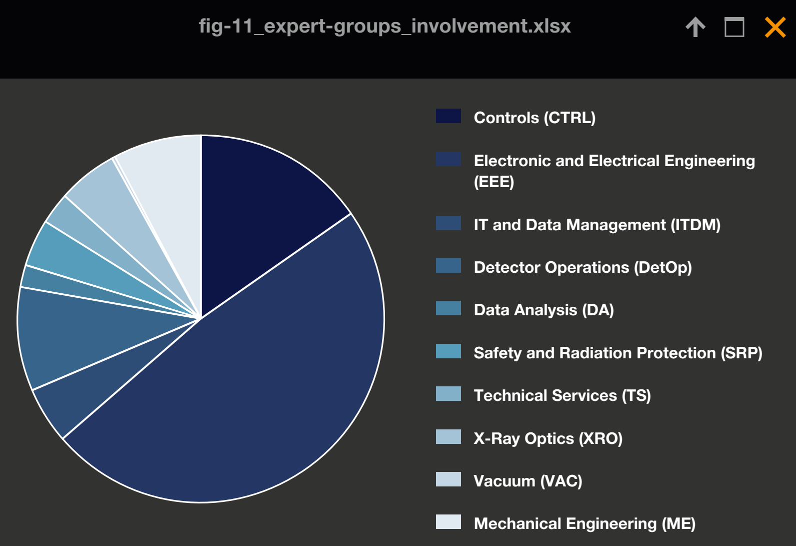


Figure 11:
Relative involvement based on working days of various expert groups from the Development and Operations Division in the DPs in 2021. Not shown is the effort by the requesting group, in the case of groups from the Experiments Division or the Administration.

Company Development

European XFEL has now faced the spread of COVID-19 for two years and has had to cope with severe changes in day-to-day business as well as user operation.

From the very beginning—in the first week of March 2020—a COVID-19 Task Force was set up to discuss organizational and operational issues related to the pandemic. A regular task force meeting was invoked with the managing directors and representatives from PR, HR, Technical Services, IT and Data Management, the User Office, Safety and Radiation Protection, the Operation Board, and the Works Council. The task force continues to advise the managing directors and meets at least once a week.

During the entire period, the regulations provided by the local authorities and the German government were strictly followed. European XFEL has implemented its own procedure to be immediately informed about potential infections and to trace suspected COVID-19 infections of staff members. Until the time of this writing, no infection chain was reported and infected staff members were able to isolate quickly if they were on campus; most already worked from home. The hygiene and distancing rules in place provided protection to staff members, who acted responsibly during the pandemic.

The year 2021 began with a lockdown imposed by the German authorities, and the annual winter break had to be prolonged until 31 January 2021. Staff presence on site had to be limited to staff members required for critical maintenance tasks and preparations for upcoming user operation. Use of offices was reduced to one person per office at a time, and the obligation to wear masks was continued. European XFEL access rules were adapted and, after the legal basis was provided by the German authorities, the campus was bound to vaccination, recovery, and testing rules (so-called “3G” rules). A new electronic access control system was implemented quickly and supported by the gatekeepers for some special cases and for external contractors and guests.

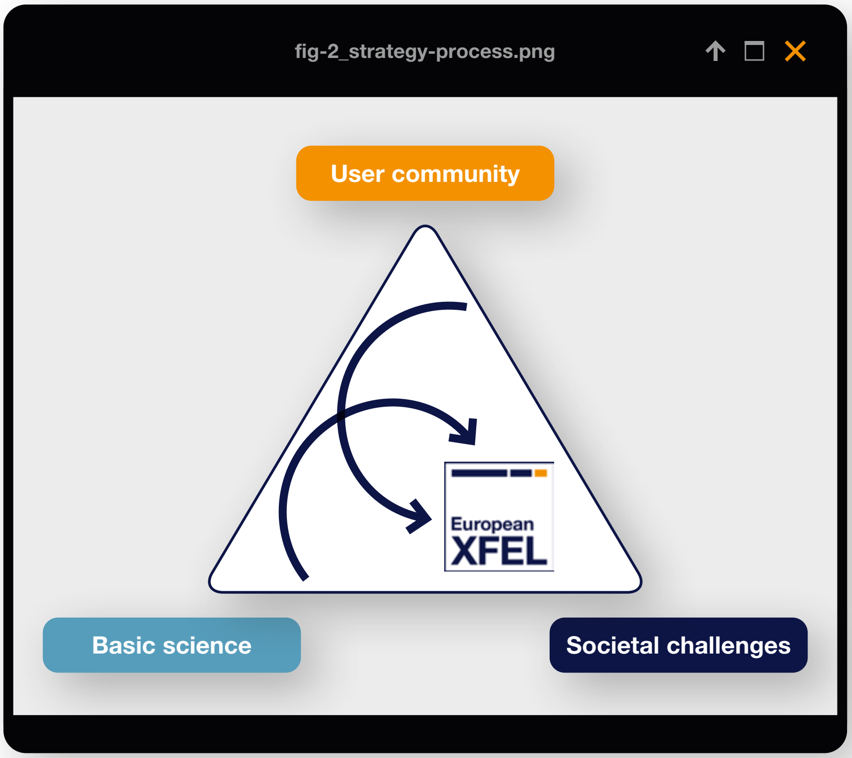
The company restaurant BeamStop stayed open during the whole year but offered only take-away meals for staff members during lockdown periods.

The safety measures on site were further strengthen by implementing the obligation to wear surgical or FFP2 (or equivalent) face masks, which were distributed by the company to staff members. Special attention was given to provide safe working conditions, especially in the experiment hutches, where close proximity between

fig-1_strategy-2030-plus.eps

fig-1_note.txt

Figure 1:
Strategy process



staff members could not be avoided. Through the combination of limited room occupancy, clear mask rules, and remote participation in experiment setups and shifts, the risk of infection was minimized.

In early February 2021, European XFEL went into a facility restart phase to prepare for user operation. For March and April 2021, only COVID-19–related experiments at the SPB/SFX instrument were planned to be conducted, which is why X-ray delivery could be restricted to SASE1. Further user experiments were scheduled for all instruments from May 2021 onward, but the participation of users on site was still strictly limited and remote participation common.

As an additional safety precaution, European XFEL started to implement a testing strategy for presence on site from mid-April onward. For this, self-test kits were provided to staff members, which allowed them to conduct rapid antigen self-tests before coming onto the premises, thereby further reducing the risk of undetected infections.

From June 2021 onwards, European XFEL was also able to offer COVID-19 vaccinations to staff members, administered by the company doctor in collaboration with the DESY medical service. This was much appreciated by staff members, particularly the simplified access to vaccination for non-German citizens. Since summer 2021, the facility slowly opened up, and staff members could work on site again. In addition, social meetings outside were made possible during the summer months and showed the interest of staff members to come together in person again. Limited business travel of staff members was also allowed within the German travel rules.

The progress of the national vaccination campaigns in combination with the wide availability of testing options enabled European XFEL to accept and welcome more users on site again. Users and external collaborators have come on site and—if needed—have stayed at the guest house. Also, guided tours through the campus and experiment hall have been restarted for special groups. Thus, the facility is back to nearly full user operation, and we hope for many more successful experiments and a return to normality in 2022.

Besides coping with and controlling the pandemic, two other topics for the future development of the facility were of particular importance in 2021.

First, the aim to “evaluate potential actions […] to mitigate the impact of the transformation from a share- to a usage-based operation cost repartition” was established by the European XFEL Council in November 2019. Since April 2020, a working group has developed a model for a concept to mitigate fluctuations in the annual operation cost contributions of shareholder countries and to balance the scientific use of the facility within a “fair return” model. Although the overall mitigation concept is still under discussion, the AFC has recommended to the Council to implement a scientific “juste retour balancing” mechanism. This tool would enable the European XFEL management to actively balance the annual shareholder contributions to the operation budget and the scientific use of the facility to a certain extent, while respecting scientific excellence as the paramount principle of providing beamtime. The Council discussed this favourably in its meeting in June 2021 and approved a pilot phase to demonstrate the feasibility of the method for the upcoming user run 2022-01.

Second, strategy development became a highly visible activity within the company, with numerous staff members supporting the management board to pave the way to the future. The strategy process is structured in five overarching action fields that focus on different dimensions.

Each action field (AF) is led by a European XFEL director:
- AF1: Operation (Sakura Pascarelli)
- AF2: Scientific Excellence (Serguei Molodtsov)
- AF3: Enabling Technology (Thomas Tschentscher)
- AF4: Increasing Facility Scope (Robert Feidenhans'l)
- AF5: Company Development (Nicole Elleuche)

The AF teams from different groups prepare the definition of strategic goals for the facility to achieve in the next decade, based on facility development potential, scientific trends, megatrends, and user needs. The strategy process aims to set the basis for an organizational transformation that adds a challenge-driven science type of operation to the discovery-driven science currently performed at European XFEL in order to actively contribute to targeted societal challenges with pivotal scientific output.

The AF teams break down the defined strategic goals into concrete activities and corresponding stakeholders. They establish specific metrics (SMART goals and indicators: specific, measurable, achievable, relevant, and time-bound) to measure the progress made on the strategic goals of the facility. The work of the AFs prepares the implementation phase of the strategy and will be concluded in a Strategy Design Report, expected by fall 2022.

A strategy board—which includes the members of the management board, the department heads, and the leading instrument scientists—ensures a coordinated and concerted effort across the AFs and acts as a forum for discussion and investigation, vetting the major directions for European XFEL in the coming decade. It also sets priorities and will condense the results in the Strategy Design Report.

In June 2021, 355 European XFEL and DESY employees took part in an interactive online “strategy flash” that created awareness for the strategy process and provided an opportunity for all staff members to give feedback and voice ideas.

In February 2022, the Strategy 2030+ was presented and positively received at the Council retreat.

European XFEL Ph.D. Programme

The European XFEL Ph.D. programme aims to train the next generation of scientists in X-ray FEL science areas, thereby disseminating the expertise and know-how acquired at European XFEL to other scientific institutions and society. Working as supervisors in the Ph.D. student programme enables scientists and engineers from all of our divisions to strengthen their research activities by broadening their scientific goals and increasing productivity. It also provides a means to improve their skills in supervision and mentoring.

Although European XFEL started employing Ph.D. students in 2014, it was only with the start of operation of the scientific instruments in 2017 that the number of Ph.D. students performing research at the facility began to increase, reaching a total of 19 Ph.D. positions in September 2019. In April 2020, a formal Ph.D. programme was launched, with the goals to strengthen student supervision, to establish a closer link to universities, research institutes, and other facilities, and to enhance long-term identification of our alumni with European XFEL.

Ultimately, the Ph.D. programme is expected to become one building block for the development of a strong in-house R&D programme—the foundation on which all successful user facilities grow and flourish.

The programme focuses on providing Ph.D. students with careful supervision and a set of courses and workshops covering scientific and technical subjects as well as soft skills. A Ph.D. committee, composed of scientists and administrative staff at European XFEL, is in charge of supervising the programme. Each Ph.D. student has a local supervisor at European XFEL and a tutor. The first leads the student in scientific and technical issues, while the latter follows up the process and provides advice, if required.

The curriculum of the Ph.D. programme is to be published soon. It includes scientific and technical courses (basic knowledge of X-ray optics, detection, beamline alignment, data analysis, etc.) and soft-skill courses, which aim to improve students' presentation and writing skills and help them to prepare for recruitment interviews, project management, conflict resolution, etc. The HR group is strongly involved in the career development of the Ph.D. students as well. In addition, European XFEL organizes a number of workshops, presentations, and courses, such as the annual Freiberg Lectures (one week in September), the weekly Photon Science Meetings, and the bi-monthly European XFEL Science Seminars, all of which are mandatory for our students.

The Ph.D. programme currently includes 52 Ph.D. positions and is very diverse, with students of more than 15 different nationalities (Figure 2).

The country of affiliation of Ph.D. students at European XFEL is shown in Figure 3.

fig-1_PhD-Zoom-meeting.mp4

Figure 1:
Ph.D. students during Zoom meeting

fig-2-4_nationalities-affiliation.xlsx

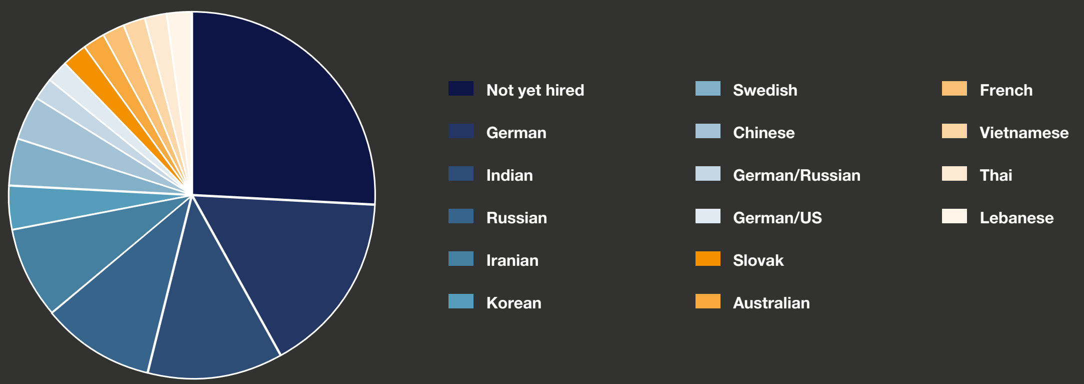


Figure 2:
Nationalities of Ph.D. students at European XFEL

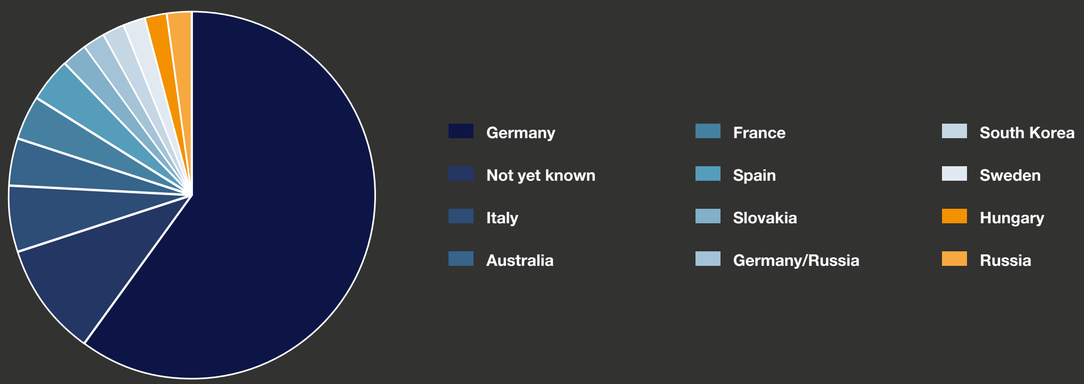


Figure 3:
Country of affiliation of Ph.D. students at European XFEL

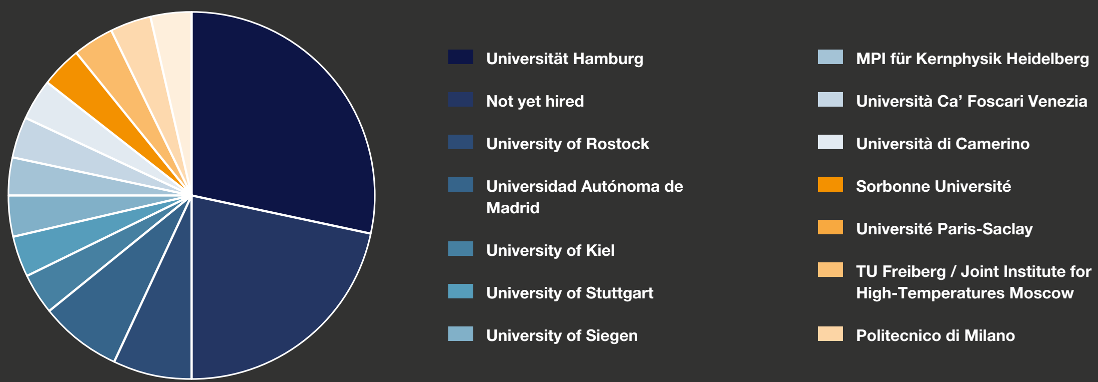


Figure 4:
Affiliations of first-year Ph.D. students

In line with our strategic goal of widening our user community, we are more proactively encouraging our staff members to establish scientific collaborations with academic groups in all shareholder countries. An important tool here is the implementation of “shared” Ph.D. student projects, with European XFEL and the partner institutes sharing the costs of recruitment. This tool has been used very efficiently, as shown in Figure 4, which illustrates the diversity in affiliations of the first-year Ph.D. students.

Finally, Figure 5 illustrates the distribution of funding sources for the first-year students. Almost 50% of Ph.D. students are covered by our R&D funds, and about 25% are “shared” with collaborating institutes.

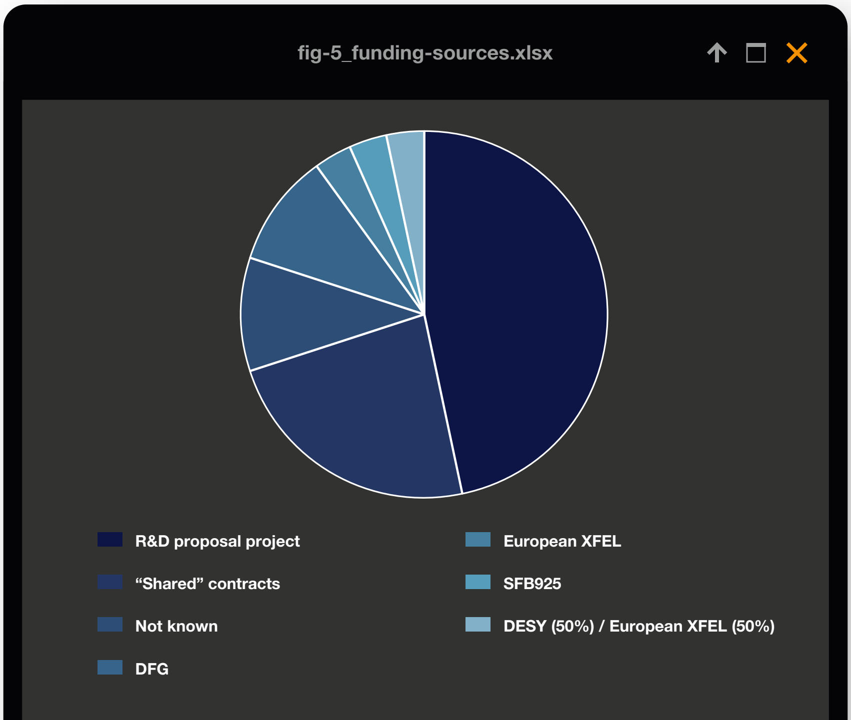


Figure 5:
Funding sources of first-year Ph.D. students

Values

The European XFEL values—collaboration, excellence, transparency, and trust—are what make the company unique as an organization. The values are at the heart of the mission and strategy. They are helping to build a supportive, inclusive, and highly motivating working environment that enables every staff member to deliver excellence.

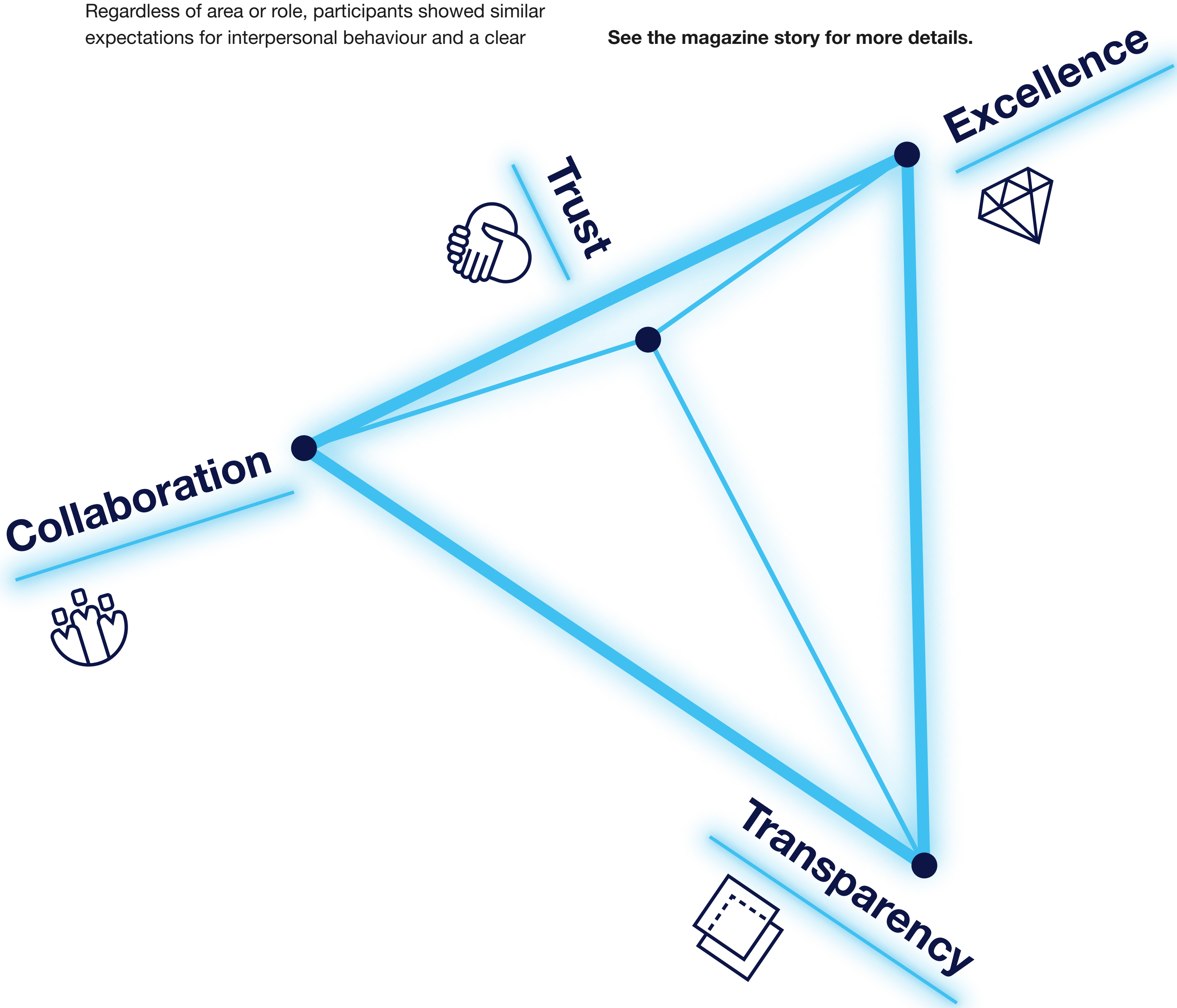
The process used to identify these values demonstrates how the whole can be greater than the sum of its parts. In a facility-wide questionnaire conducted in June 2021—in which 70% of staff members took part—participants gave suggestions for improving the company culture and defining our company values.

Regardless of area or role, participants showed similar expectations for interpersonal behaviour and a clear sense of what motivates and drives us. This does not mean that all have exactly the same values but that there is common ground.

The values link directly to implementing the Strategy 2030+ and delivering the European XFEL mission by stating what is important to the company and how staff members should treat one another, users, and other stakeholders.

As a further measure, a communication campaign was launched to make the values visible. In addition, a network of "culture change agents", composed of staff members from different functional areas, was created. The mission of this network was to increase awareness of the company values.

See the magazine story for more details.



Budget and Third-Party Funding

Budget

At the end of 2021, 98.6% of the European XFEL construction budget was spent. The annual operation budget was 137.3 million euro (M€) in 2021 and will increase to 140.7 M€ in 2022.

Parallel to the 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.

An important change to the budget structure of European XFEL is related to the new capability to prepare for future big investments by creating an “indicative” budget through the pre-allocation of operation funds. The indicative budget is now reported as part of the newly established Facility Development Programme, describing and showing the planned expenses and their relation to the future-oriented development of the facility, including strategic activities and contingency plans.

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 2021 amounted to 145 M€. Of this, 137 M€ (95%) was related to operation and 8 M€ (5%) was allocated to ongoing construction projects.

Recurrent and capital costs were the largest part of the costs and totalled 74 M€ (51%). Another 66 M€ was spent on personnel, including staff from DESY. A further 6 M€ was allocated for smaller upgrades.

For 2022, an increased annual payment operation budget of 140.7 M€ was approved by the European XFEL Council and a further 11.1 M€ for the finalization of the construction phase.

fig-1_Payments-by-major-activity.xlsx

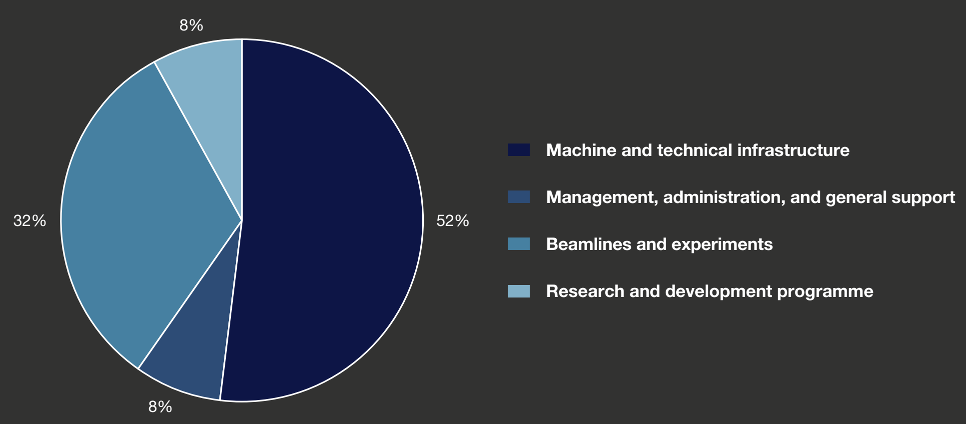


Figure 1:
Payments by major activity in 2021

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—within the framework of its Horizon 2020 and Horizon Europe research and innovation programme—and the German Research Foundation (DFG) are examples of the types of prestigious funding bodies making these contributions, underlining the high quality of research projects performed by European XFEL scientists.

Third-party funding

In 2021, European XFEL participated in 15 research projects, eight of which were funded by the EU Horizon 2020 and Interreg programmes, and six by national funding organizations, such as DFG and the German Federal Ministry of Education and Research (BMBF).

The overall income from these projects was 1.1 M€, of which 67% came from European and international funding and 33% from national funding. The funds spent by third-party projects amounted to about 0.9 M€ in 2019, 1.1 M€ in 2020, and 1.3 M€ in 2021.

In 2021, nine staff members were employed exclusively for third-party–funded projects, five of these projects ended, and six new projects were started.

Call for R&D projects by European XFEL and DESY staff

In February 2021, European XFEL issued its third call for photon-based R&D proposals, open only to the staff of European XFEL and DESY. In these special calls, staff members of the two institutions can apply for funding over three years for R&D projects related to the development of the European XFEL facility, possibly realized in cooperation with groups at other scientific institutions, in particular in the shareholder countries.

However, the COVID-19 crisis, with associated lockdowns worldwide and onsite restrictions, severely affected the progress of R&D projects from the two previous calls (issued in 2019 and 2020), with many deadlines and associated payments postponed. In addition, a number of Ph.D. student projects were delayed, leading to a record number of Ph.D. students enrolled in the European XFEL Ph.D. programme (close to 40 at that time).

Notwithstanding this critical situation, in launching the R&D call 2021 (for the projects to be conducted in 2022), European XFEL wanted to provide staff with an opportunity to further develop the in-house research programme, drive strategic developments, and keep the facility at the forefront of research and innovation worldwide.

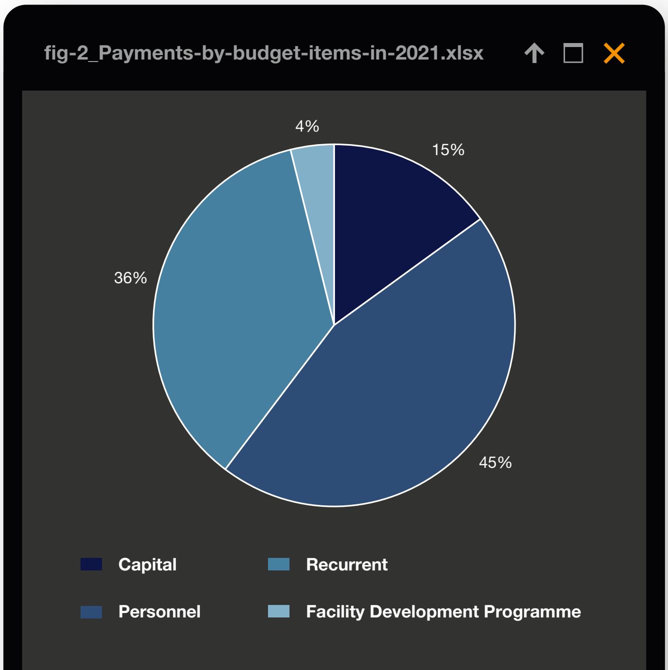


Figure 2:
Payments by budget items in 2021

Due to the high amount of ongoing commitments in many European XFEL and DESY groups at the beginning of 2021, reduced demand for R&D funds was expected. Therefore, the budget was reduced by more than 1.5 M€/year to 6.8 M€ in total for three years, corresponding to roughly half of the amount allocated in the R&D call 2020 (Table 1).

A special focus for the R&D call 2021 was on scientific collaborations with new groups or with groups from underrepresented shareholder countries that would be particularly valuable to the development of the facility. This included joint Ph.D. students enrolled at universities in these countries.

Seventeen applications were received, covering a broad range of topics. Out of these, 16 proposals, well distributed over two European XFEL divisions, and some including DESY colleagues, were approved (Figure 3).

A total of 7.7 M€ in funding was requested, far more than could be granted. Sixteen proposals were awarded funding but were partially adjusted in terms of funding or scientific scope. Most projects will run for a maximum of three years and will have an annual budget of up to 300 k€. The majority of the projects will start in 2022 with a total funding of 2.3 M€ for the first year. The total budget for all the projects covering the full funding period amounts to 6.8 M€.

fig-3_R-D-funding-distribution.xlsx

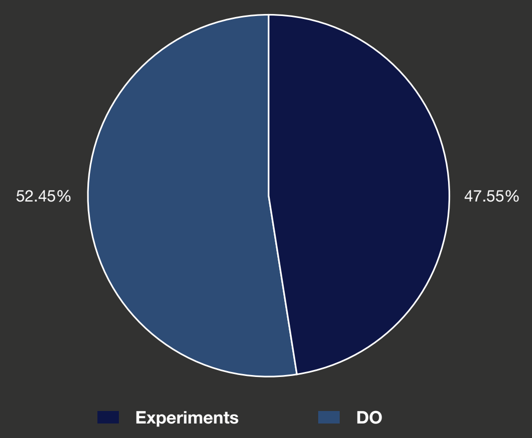


Figure 3:
Funding distribution for R&D projects in the Experiments Division and the Development and Operations (DO) Division

Table 1: Calls for R&D funds (2019 to 2021)

	2019	2020	2021
Deadline	May 2019	May 2020	April 2021
Selection	July 2019	July 2020	May 2021
Allocation	September 2019	July 2020	July 2021
Number of submitted proposals	32	30	17
Number of approved proposals	11	28	16
Allocated budget	4.4 M€ over three years	11.2 M€ over three years	6.8 M€ over three years
Allocated FTEs	11–15 FTEs/year	25–28 FTEs/year	15.5–17.5 FTEs/year

Managing Quality, Safety, Risk, and Customs

Quality management
In 2021, overall improvements in quality management—comprising different quality-oriented services, procedures, and guidelines—resulted in tangibly optimized processes and procedures. In addition, new areas were identified on which European XFEL needs to focus in the next years. The optimization potential and adjustments are mostly connected to the maturing of European XFEL and related, specific requirements as well as to some changes in the legal framework the company has to follow.

One example is the development and implementation of the new European XFEL procurement rules, which were drawn up together with the shareholder countries and were subject to Council approval. As part of these new rules, European XFEL will engage more intensively with the national industrial liaison offices and address companies and suppliers from the shareholder countries for particular tender procedures or other purchases, whenever legally possible and in line with the corresponding awarding regulations.

Environmental sustainability is one aspect that European XFEL needs to focus on in a more structured and coordinated way. Some related actions have already been taken. For example, the warehouse and logistics team has been re-using supplied transport boxes and packaging materials—another contribution to the sustainable use of resources. New trends in corporate sustainability, the expanding climate crisis, lightning-speed growth in cleantech, and rising interest from many stakeholders and European XFEL shareholders will make environmental sustainability a management priority in the coming years.

Our activities—which are supported by regular internal audits and an external end-of-year audit—aim to combine 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 we established and the procedures we implemented or adapted in 2021 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.

A major, ongoing quality management activity is the implementation of an enterprise resource planning (ERP) system. Mainly due to the pandemic, the project was delayed, and the first instance—with some main modules focusing on financial/budget management, controlling, and procurement—will be rolled out in 2022. Within the project “HR 2.0 – Next Generation HR IT”, which was launched in 2021, another ERP module will be added in 2024 to significantly optimize and simplify personnel and working-time–related processes.

Safety and radiation protection
In 2021, the number of work accidents was again significantly smaller than in pre-pandemic years. There were no accidents in 2021 leading to long-term effects, as shown in Table 1.

Accidents

	Minor	Declared	Commuting	Total
Q1	4	0	2	4
Q2	3	0	0	3
Q3	6	2	3	8
Q4	4	0	0	4

tbl-1_note.txt

Table 1:
Number of work accidents during each quarter of 2021. Declared accidents are those resulting in an absence of more than three working days. All other accidents are considered minor. Commuting accidents can be minor or declared.

Figure 1:
Personal protective materials against the COVID-19 pandemic

One of the key responsibilities of European XFEL towards its staff members, users, and guests is to train them in workplace risk management. Many of these training sessions happen face-to-face, but online training is becoming increasingly important. The current online training platform will be replaced in 2022 by a new, reliable, and robust system that will significantly reduce the need for maintenance and support. Currently, the new training system is being interfaced to the access control management system at European XFEL. The online training material has also been completely revised.

Risk management

In February 2021, European XFEL launched a web-based risk management system (RMS). This customized tool was developed together with a company in Poland. All technical and scientific group leaders were introduced to the system in the first quarter of 2021. Directors and department heads followed in summer 2021.

The introduction and use of the RMS led to more active risk management within all involved groups. The RMS allows reports to be created within minutes and has changed risk management at European XFEL. Risks are evaluated by the groups and reported to the risk coordinator and the risk committee. Centrally required resources were reduced and, at the same time, the awareness of and active risk management in the groups increased. Risk reports will be written every half-year, based on the calendar year, and shared with the European XFEL Administrative and Finance Committee (AFC) and Council.

Customs and export control

In a globalized world, export control is important not only in the private sector but also in science and research. To meet these requirements, a new Customs and Export Control Office was established.

The office takes care of all customs-relevant processes (import and export of goods as well as export-legal assessment of technical support) and has significantly improved them. All German, EU, and US customs and export regulations are taken into account, and other country-specific regulations are applied on a case-by-case basis. The benefits include faster processing of all import and export procedures, which is particularly important for the timely arrival of samples for experiments, safe shipping of high-quality equipment abroad for repair, and avoiding incorrect customs declarations leading to delays, heavy fines, or even confiscation of the goods.

International Collaboration

As an international facility, European XFEL maintains extensive collaborations with partners around the world, especially with scientists and institutes in its shareholder countries. In 2021, despite the COVID-19–related travel restrictions that still prevented most meetings in person, the opportunities for online exchange were fully exploited to enable close communication with scientific communities.

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

- **ATTRACT 2** (GA No. 101004462)
  Breakthrough Innovation Programme for a Pan-European Detection and Imaging Eco-System – Phase 2

- **CALIPSOplus** (GA No. 730872)
  Convenient Access to Light Sources Open to Innovation, Science and to the World

- **CREMLINplus** (GA No. 871072)
  Connecting Russian and European Measures for Large-scale Research Infrastructures

- **EDAX** (GA No. 669531)
  Beating Complexity through Selectivity: Excited state Dynamics from Anti-Stokes and non-linear resonant inelastic X-ray scattering

- **LEAPS-INNOV** (GA No. 101004728)
  LEAPS pilot to foster open innovation for accelerator-based light sources in Europe

- **MS SPIDOC** (GA No. 801406)
  Mass Spectrometry for Single Particle Imaging of Dipole Oriented protein Complexes

- **PaNOSC** (GA No. 823852)
  Photon and Neutron Open Science Cloud

Within the Röntgen–Ångström Cluster (RÅC), the InVision project was continued as a Swedish–German research collaboration in the fields of materials science and structural biology. Researchers from Lund University in Sweden, TU Berlin in Germany, and European XFEL aim to improving the understanding of the dynamics of metallic foams and granular matter using sub-microsecond single-shot multiprotection X-ray imaging.

With the adoption of a "European Strategy on the Digital Transformation of Accelerator-based Photon Sources towards a resilient and sustainable European Research Area" (Digital LEAPS), the LEAPS consortium (League of European Accelerator-based Photon Sources) shows a new pathway of the LEAPS facilities into the post-COVID-19 era. With a structured programme of three main pillars (LIP, HR4, and Star), in which European XFEL is an active contributor, new technologies and approaches will be developed for remote user operation, digital communication and training, resilient and energy-saving operation, AI-assisted molecular infection fighting, and advanced materials for digital transformation and circular economy.

In April, the joint Horizon 2020 project LEAPS-INNOV was launched, focusing on the implementation of new strategies and activities for long-term partnerships between industry and the European light sources, synchrotrons, and free-electron lasers, with their tens of thousands of users.

European XFEL—together with its partners at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) and DESY—celebrated the inauguration of the Helmholtz international Beamline for Extreme Fields (HiBEF) on 31 August 2021, welcoming to campus high-ranking representatives from politics and international partners. This was a much-appreciated opportunity for direct exchange that fostered connections between scientific

collaboration-logos_01.eps

collaboration-logos_02.eps

fig-1_HiBEF-inauguration.JPEG

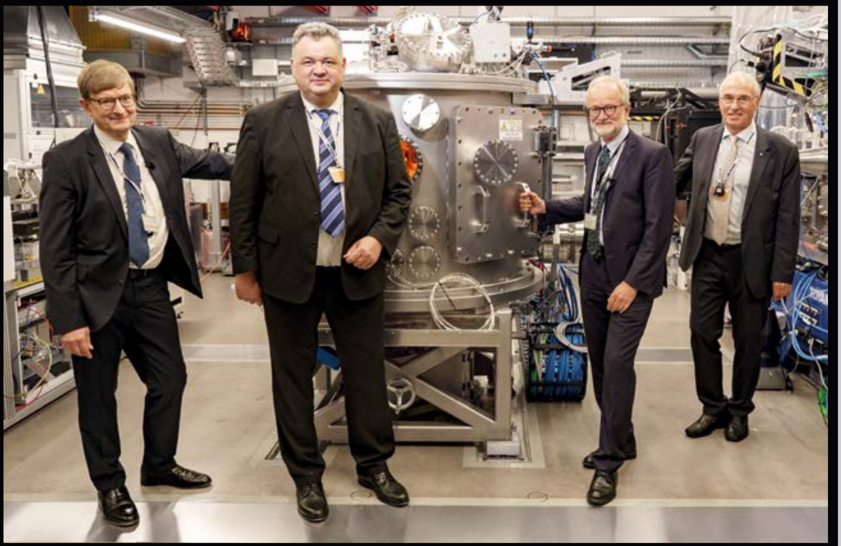


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Figure 1:
Otmar D. Wiestler (President of the Helmholtz Association), Sebastian M. Schmidt (Scientific Director of HZDR), Robert Feidenhans'l (Chairman of the European XFEL Management Board), and Helmut Dosch (Chairman of the DESY Board of Directors) during the official HiBEF inauguration after the Interaction Chamber 2 was pushed into the beam at the HED scientific instrument.

and political partners and helped enable the realization of this cutting-edge infrastructure at European XFEL.

European XFEL is also a member of EIROforum, a partnership of eight European intergovernmental research institutes, providing a platform for regular exchange and joint events, also reaching out to other organizations. On 13 January 2021, EIROforum met with the National Laboratories Director's Council (NLDC) to discuss areas of stronger collaboration, including the scientific response to the COVID-19 pandemic. As a result of this exchange, a joint workshop was organized in the context of the UN Climate Change Conference of the Parties (COP26) in which approaches were discussed to address the climate crisis (e.g. by reducing the carbon footprint and ensuring a more sustainable operation of research facilities). For the first time in two years, EIROforum representatives were also able to meet in person for their biannual Director General Assembly, which was hosted by ESRF in Grenoble.

fig-2_note.txt

Figure 2:
On 23 June 2021, Serguei Molodtsov (upper right) was appointed as the new FELs OF EUROPE Chairman for the next two years.

Within the Baltic Science Network initiative (BSN), European XFEL continued its support for this initiative, led by the Hamburg Ministry for Science, Research, Equalities and Districts (BWFGB), which aims to generate new scientific collaborations within the Baltic Sea region in both academia and industry. The BSN_powerhouse project held its final videoconference in June 2021. One major outcome was that a continuation of the initiative is highly desired, also to gather more new users for research facilities such as European XFEL and DESY. Within this LaunchPad initiative, European XFEL leading scientists and experts were involved in two of the four projects that were awarded funding for coaching activities in order to further develop the projects.

European XFEL is also part of the Hanseatic League of Science (HALOS), a project fostered within the European Regional Development Fund Interreg Öresund-Kattegatt-Skagerak (ÖKS) programme. This network, which includes researchers from Hamburg and southwestern Scandinavia, includes unique research facilities—MAX IV, ESS, DESY, EMBL Hamburg, and European XFEL—to foster life science innovation and research.

Within FELs OF EUROPE, a collaboration of all free-electron laser (FEL) facilities in Europe, European XFEL Scientific Director Serguei Molodtsov took over as chairman of the network in June 2021. The network, which includes 15 facilities in 11 countries, aims to address the technological and scientific challenges of FEL science and provide a unique pan-European research infrastructure that enables the exploitation of the full scientific potential of these accelerator-based short-pulse light sources.

With support from the project CALIPSOplus, funded by the European Union's Horizon 2020 research and innovation programme, European XFEL also hosted, together with DESY, the 16th General Assembly of the European Synchrotron and FEL User Organization (ESUO) on 18–19 October 2021, which addressed, among other topics, the transition of ESUO to become an international non-profit organization (AISBL under Belgian law) and the LEAPS-ESUO strategic partnership. The elections of the new ESUO President and Executive Board took place during the meeting.

To support the education and training of the next generation of FEL students, European XFEL also participated in the annual HERCULES European School of Neutrons and Synchrotron Radiation for Science, which took place between 22 February and 26 March 2021, as well as the RACIRI 2021 Summer Lecture on 24 August 2021.

European XFEL also contributed to national workshops organized by the synchrotron radiation and FEL science communities of shareholder countries—such as France, Italy, Denmark, Russia, and Spain—in order to stay in close contact with the corresponding user communities and engage with current and new user groups.

To build up new connections and strengthen already existing collaborations with partner institutions in Russia, European XFEL joined a virtual meeting series coordinated by DESY with Russian research institutions.

Accompanying the substantial progress made towards Spain becoming a full shareholder of European XFEL, Managing Director Robert Feidenhans'l visited the Madrid Institute for Advanced Studies in Nanoscience (IMDEA Nanociencia) to sign a collaboration agreement to strengthen scientific ties between both institutions and help to promote X-ray FEL science in Spain. The visit also included meetings with representatives of the Spanish Ministry of Science and Innovation as well as the Center for Energy, Environmental and Technological Research (CIEMAT).

fig-3_note.txt

Figure 3:
Robert Feidenhans'l and Cristina Palencia visited the IMDEA Nanociencia premises in Madrid in November. Wojciech Gawelda (former FXE scientist at European XFEL), Rodolfo Miranda (Director of IMDEA Nanociencia), Fernando Martin and José Manuel Martín García (regular European XFEL users), and prominent IMDEA scientists met to discuss collaboration opportunities between both institutions.

fig-3

Contacts to Industry

In 2021, an important achievement of the European XFEL Industrial Liaison Office (ILO) was the establishment of continuous and successful collaboration with the national ILOs of the shareholder countries, aimed at supporting the procurement and development of state-of-the-art technologies. In addition, European XFEL started to include innovation-driven companies in the experiment programme, which is one of the main objectives of European XFEL ILO.

European XFEL has involved the 12 national ILOs of the shareholder countries in a new process that enlarges the pool of potential suppliers and industrial collaborators for our staff. National ILOs serve as country representatives and are comprised of experts with relevant networks of companies as well as research and technology organizations. The process, coordinated by European XFEL ILO as outlined below, allows access to a large network of companies in the shareholder countries in the business of cutting-edge components and state-of-the-art services.

The main points of the cooperation are as follows:

- The 12 national ILOs are informed about newly published open calls for tender in order to promote participation in their industrial network and increase the number of tenders, which offers a clear advantage for European XFEL.
- European XFEL ILO involves the national ILOs directly to search for technology providers, based on the needs of our R&D projects and long-term innovative developments. Moreover, European XFEL ILO analyses, on a yearly basis, the industrial collaborations and previous procurements in order to foresee future technology trends. Scientific staff members are continuously kept up to date on the latest technology that can support their development and offer innovative solutions.
- The 12 national ILOs are involved not only in procurement processes or industrial collaborations but also in other industry-related topics, such as finding providers of courses for CE marking, locating potential industrial users, or raising third-party funding in bilateral cooperation between countries.
- Two national ILO meetings were organized by European XFEL ILO in 2021 to discuss improvements of processes and specific aspects of the newly approved European XFEL procurement rules.

To promote industrial collaboration with our company, European XFEL ILO supported the organization of the Big Science Business Forum in Granada, Spain, which had to be postponed until 2022. The event will bring together key suppliers and high-level representatives of various international science institutes, including European XFEL, to explore new possibilities for advancing the development of novel technologies. Moreover, a temporary

fig-1_note.txt

Figure 1:
Innovation comes in many forms. This non-coplanar Bragg magnifier (patent pending) was invented by Roman Shayduk. The MID instrument scientist led an award-winning R&D project to develop a prototype of a channel-cut crystal monochromator, inspired by his invention.

fig-1_2022-02-11_IMG_2113.tif

Figure 2:
Visualization of the national ILO network: The participating countries work together with European XFEL ILO to promote innovation and collaboration.

innovation marketplace will be set up in order to foster technology transfer. Webinars were organized in 2020 and 2021, while attendees waited for the in-person conference to take place. In particular, a virtual event was organized with the direct support of European XFEL ILO in February 2021 to inform about and promote the technology transfer track programme that will be held during the in-person conference in 2022.

European XFEL ILO also supports innovation "in the making". It fosters the realization of state-of-the-art systems using third-party funding and supports applications, for instance to the Horizon Europe programme, by anticipating outcomes in applied science and their impact on the industrial world. Through technology trend analysis, European XFEL ILO demonstrates the role of the proposed projects as avant-garde in the European and worldwide context. One example in 2021 was the support of the Tomoscopy project, awarded by the EIC Pathfinder programme, the new financial instrument coordinated by the European Innovation Council. Tomoscopy is a three-dimensional imaging system that exploits the unique megahertz repetition rate of the European XFEL. Patrik Vagovic and Valerio Bellucci from European XFEL were supported in filing a patent that is now awaiting evaluation by the European Patent Office.

European XFEL ILO promotes the use of the facility for applied science of industrial interest in the field of structural biology by involving pharmaceutical companies. Three industrial users participated in the European XFEL experiment programme in collaboration with our staff. Two of them took part in a special call dedicated to COVID-19–related research.

Regarding knowledge and technology transfer, an innovation strategy was drawn up by European XFEL ILO and Managing Director Robert Feidenhans'l and then further developed, improved, and approved by the European XFEL Management Board.

European XFEL ILO supported instrument scientist Roman Shayduk in the first patent application by European XFEL, "Method and apparatus for X-ray beam expansion and/or compression and/or collimation and/or focusing and/or X-ray image magnification (EP3723103A1)". The patent was published after a positive evaluation by the European Patent Office.

In connection with the improvement of academia–industry collaboration and potential technology transfer, European XFEL ILO was directly involved in the innovation activities of the League of European Accelerator-based Photon Sources (LEAPS). In particular, in the framework of the EU-funded project LEAPS-INNOV, in cooperation with Elettra Sincrotrone Trieste, European XFEL ILO set up a process for knowledge and technology transfer of undulator technologies from the 16 LEAPS facilities. Furthermore, the organization of the first workshop on undulator technology, with 50 participants from academia and industry, fostered mutual exchange and collaboration opportunities.

Outreach

In 2021, outreach activities to non-expert audiences took place predominantly online. The virtual tour, which features 360° photographs and short animated films, was updated with new pictures and extended to include locations such as the European XFEL warehouse, the workshop, the BeamStop company restaurant, and the guest house. Participants in scientific events took part in virtual tours of the facility as well as onsite tours, when permitted, due to low COVID-19 infection rates in the autumn.

In addition, new videos supported communication and outreach to expert audiences. One video explained the tunnel components for X-ray optics and photon diagnostics to bachelor students as part of the HERCULES School 2021. The other was a guided tour providing details about the detectors at all six scientific instruments of the European XFEL as part of an online workshop for high school students celebrating the 20th anniversary of the online platform LEIFIphysik. Two videos were produced explaining the MID instrument: an animated video showing X-ray scattering techniques and a three-minute-long time-lapse video following the change of configuration at MID from wide-angle X-ray scattering (WAXS) to large field of view (LFOV)—a process that takes up to 18 hours. In addition, a new visual guide about the European XFEL campus was created for users visiting the facility.

One of the outreach activities for schools was an online holiday event for Young Talents (YoTa) Hamburg. It was live-streamed from the sample environment laboratories. Students were introduced to both light and electron microscopy, with opportunities to ask questions and investigate samples in detail. The comic book "Norovirus Superstar", which can be downloaded for free, gives insights into the EU-funded MS SPIDOC project and explains how the European XFEL's high-quality beam enables single-particle imaging (SPI) of individual viruses or potentially of protein complexes. Also, planning began for the facilities and programmes for the two new school labs that will be part of the visitor centre, scheduled to open in 2024. Networking with schools from the surrounding area started in order to develop an innovative teaching module on virus research for high school students.

Almost all guided visitor tours were moved online. Around 400 individual visitors attended nine guided online tours of the facility. Visitors included university students, high school classes, scientists, and local interest groups as well as the general public. Exhibits, a video

fig-1_guest-house_360.tour

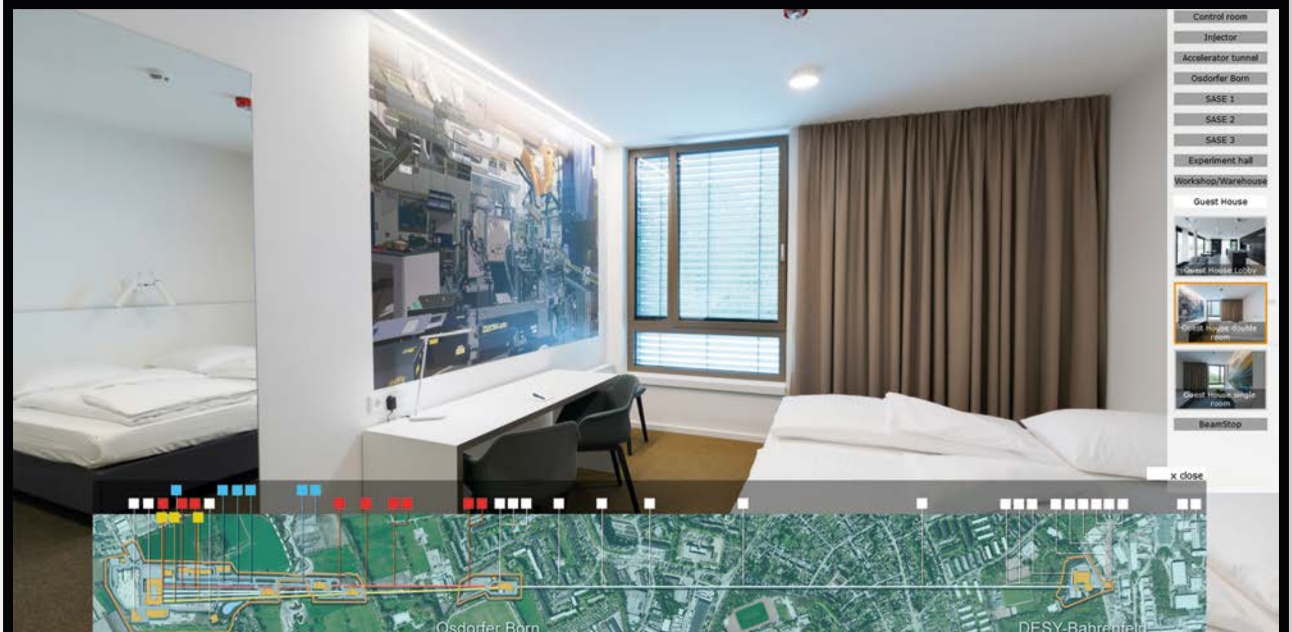


Figure 1:
The 360° virtual tour was updated with new locations, including the guest house.

fig-2_norovirus_superstar.epub

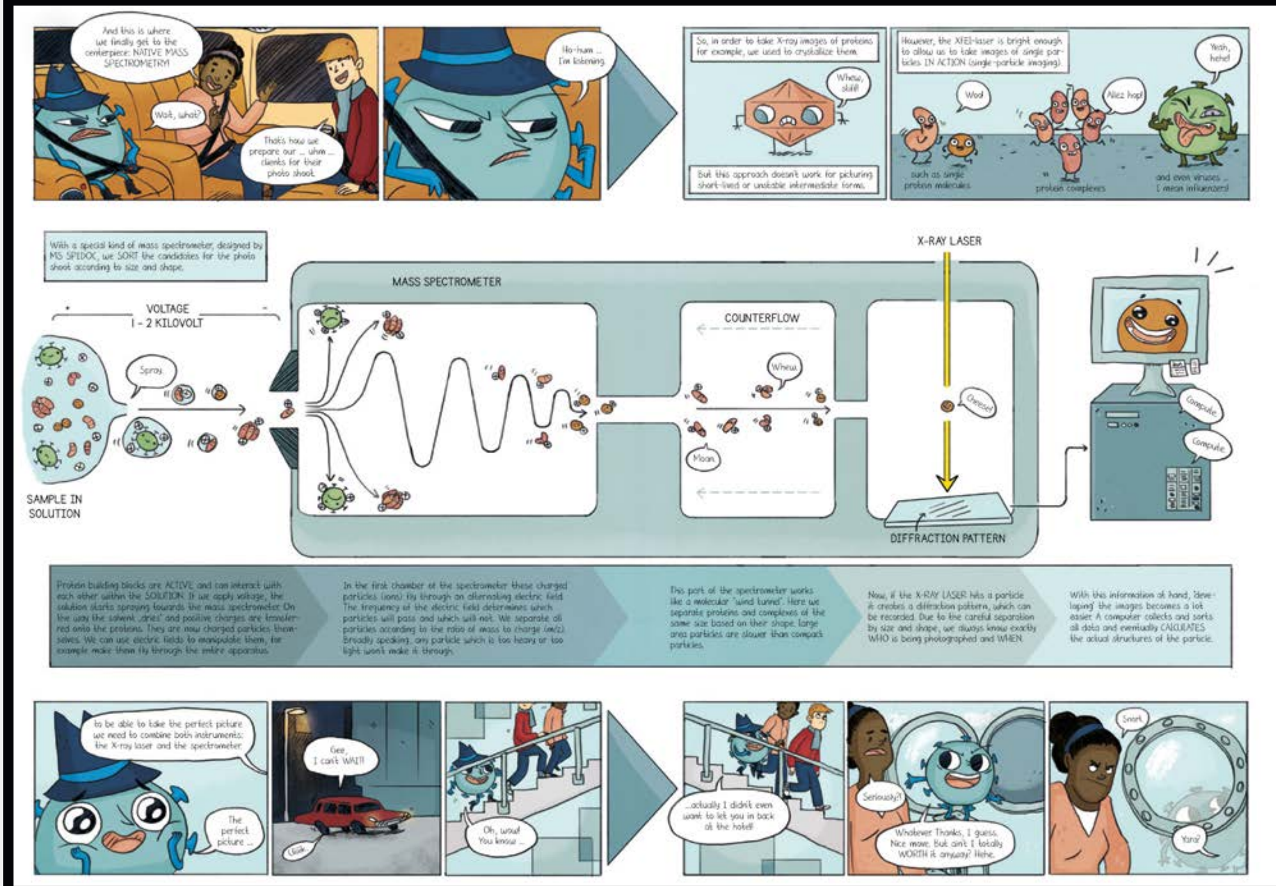


Figure 2:
The comic "Norovirus Superstar" explains how the European XFEL can be used to image single particles.

programme, and posters about European XFEL were presented at the annual science festival "Highlights der Physik" in Würzburg, Germany. Additionally, Scientific Director Thomas Tschentscher gave an evening lecture on X-ray films showing (bio)chemical reactions. Other planned events were cancelled due to the COVID-19 pandemic. Two online public lectures were especially successful: a lecture celebrating the 60th anniversary of the invention of the laser, part of the DESY series "WissensWerte", and a talk by European XFEL Data Scientist James Wrigley at the Chaos Computer Club's annual conference. Both drew a large audience.

Fourteen information panels were installed on the Schenefeld campus informing about the European XFEL facility, buildings, underground installations, and environmental compensation measures. The panels are connected by an approximately 1600 m long green line on the ground, so external visitors can easily find their way around the campus. Planning for the visitor and conference centre continued in 2021 and is at an advanced stage. The groundbreaking ceremony will take place in 2022.

Figure 3:
One of the 14 information panels of the 1600 metre long info tour

Director's Outlook

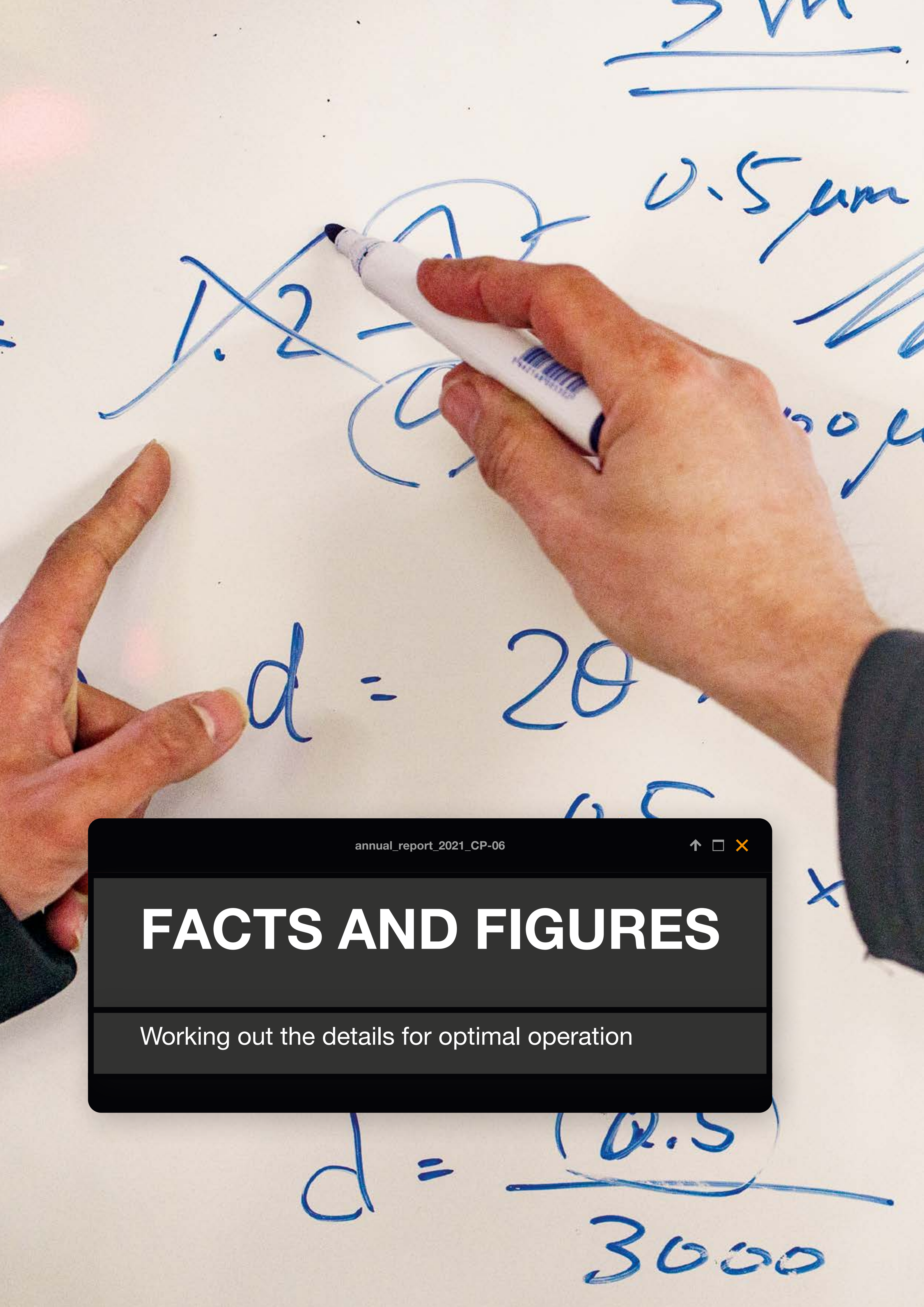
Writing an annual forecast at the beginning of the year is a challenge once again. Last year, I wrote the outlook during a lockdown, and it was not possible to predict how much the COVID-19 pandemic would affect the European XFEL operation and user programme. Fortunately, 2021 went well. This year, it is not much easier to make predictions just as the omicron coronavirus wave is reaching Germany. COVID-19 will most likely affect the user programme, but I tend to be optimistic and hope the impact will be relatively mild. Once again, major concerns are the inability of users to travel and the effect of contact restrictions on site visits as well as the possibility of more infections and subsequent quarantine among staff. I very much hope that all travel restrictions will soon be lifted and that we can again meet many users on site, not just online. Scientific progress is based on the exchange of knowledge, know-how, and skills; here, open borders play an essential role.

In 2022, the number of facility users will further increase. A great achievement in the schedule for the first half of 2022 is the amount of beamtime for the user programme: With 4940 hours and 54 user experiments scheduled, we are close to the mid-term target value planned to be achieved in 2025–2026, for which 10 500 hours of user beamtime are foreseen in a full year. That we are already getting close to this target in the first half of 2022, only five years after the start of operation, is a significant achievement by the staff of European XFEL and our colleagues at DESY. However, this increase in beamtime for users comes at the price of less time for commissioning and in-house research. It will hence be difficult to keep such a high level of user beamtime in the second half of 2022. Nevertheless, I am optimistic that there will be a significant increase in beamtime for the user programme compared to earlier years. This is also highly needed, as there is a growing interest in doing experiments at the European XFEL, as evidenced by the large amount of exciting proposals we received at the end of 2021.

Apart from the increased amount of beamtime for users and the opportunity to once again welcome users on site, I am looking forward to the first commissioning of the APPLE-X helical undulator at the SASE3 beamline. The installation in the tunnels is going well and according to plan. This will be a great step forward for our programme in research on magnetism, which we hope can lead to the development of faster and more efficient data storage. Another major step will be the first commissioning of the third port, the Soft X-Ray Port (SXP), also on the SASE3 beamline, which is planned for the second half of 2022.

I am also looking forward to meeting staff members from European XFEL and colleagues from DESY on site and in person in the spring, when most of the COVID-19 restrictions will hopefully be over. I am particularly excited to speak to our Council and committee members in person again in Schenefeld—I have missed the informal discussions and knowledge exchange with all of our committees. And I am looking forward to travelling again to our shareholder countries to meet their representatives and the user committees. Plans are in the making for travel to Slovakia, Hungary, and Poland.

I hope for a year with many people on site again and plenty of successful experiments.



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FACTS AND FIGURES

Working out the details for optimal operation


= 0.5 mm

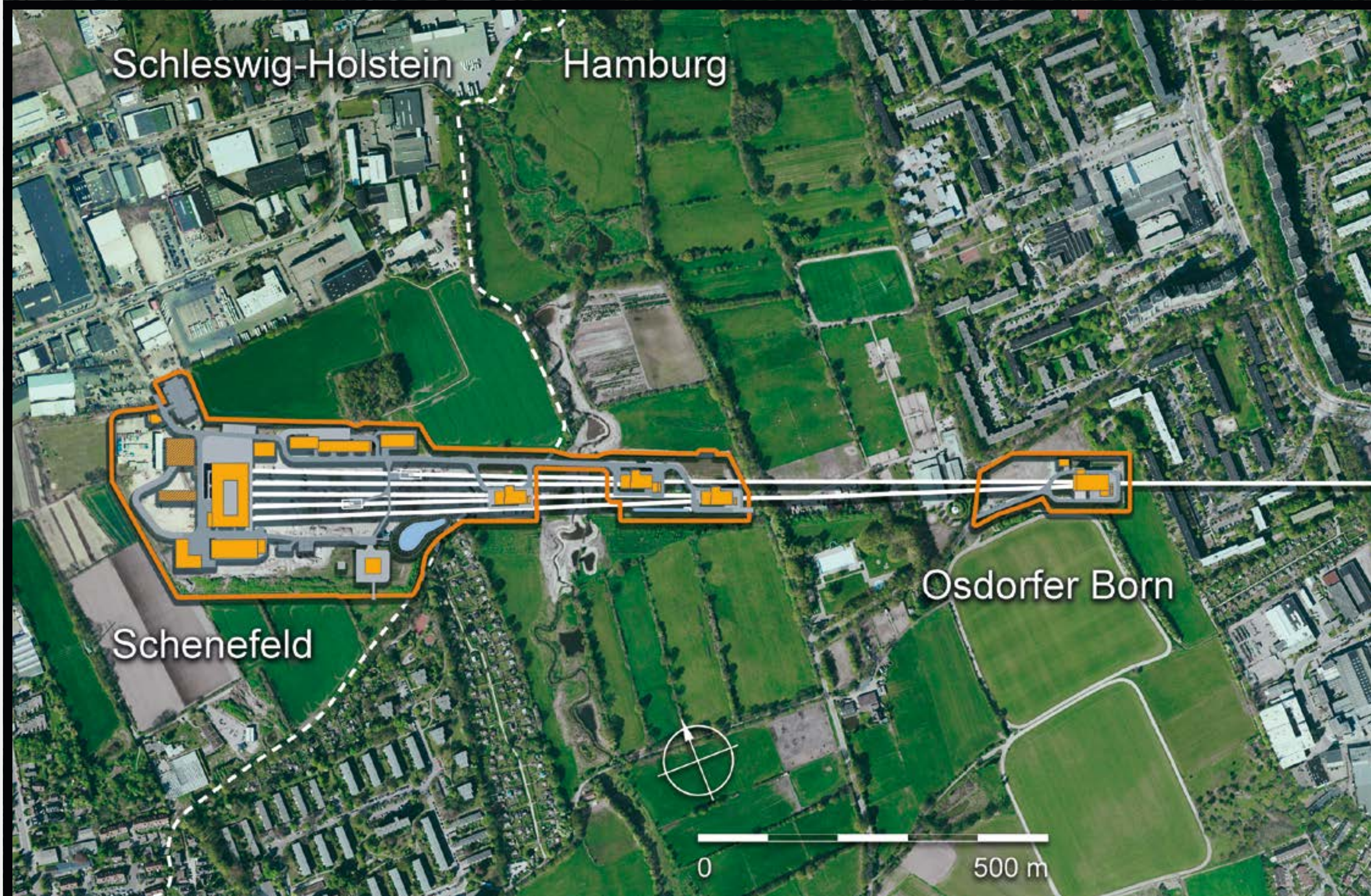
At a Glance

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

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

fig-1_eu-xfel.facility



one distribution shaft, and the Schenefeld campus site, which hosts the underground experiment hall with a large laboratory and office building on top. The latter serves as the company headquarters.

As of December 2021, 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 2021, 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.

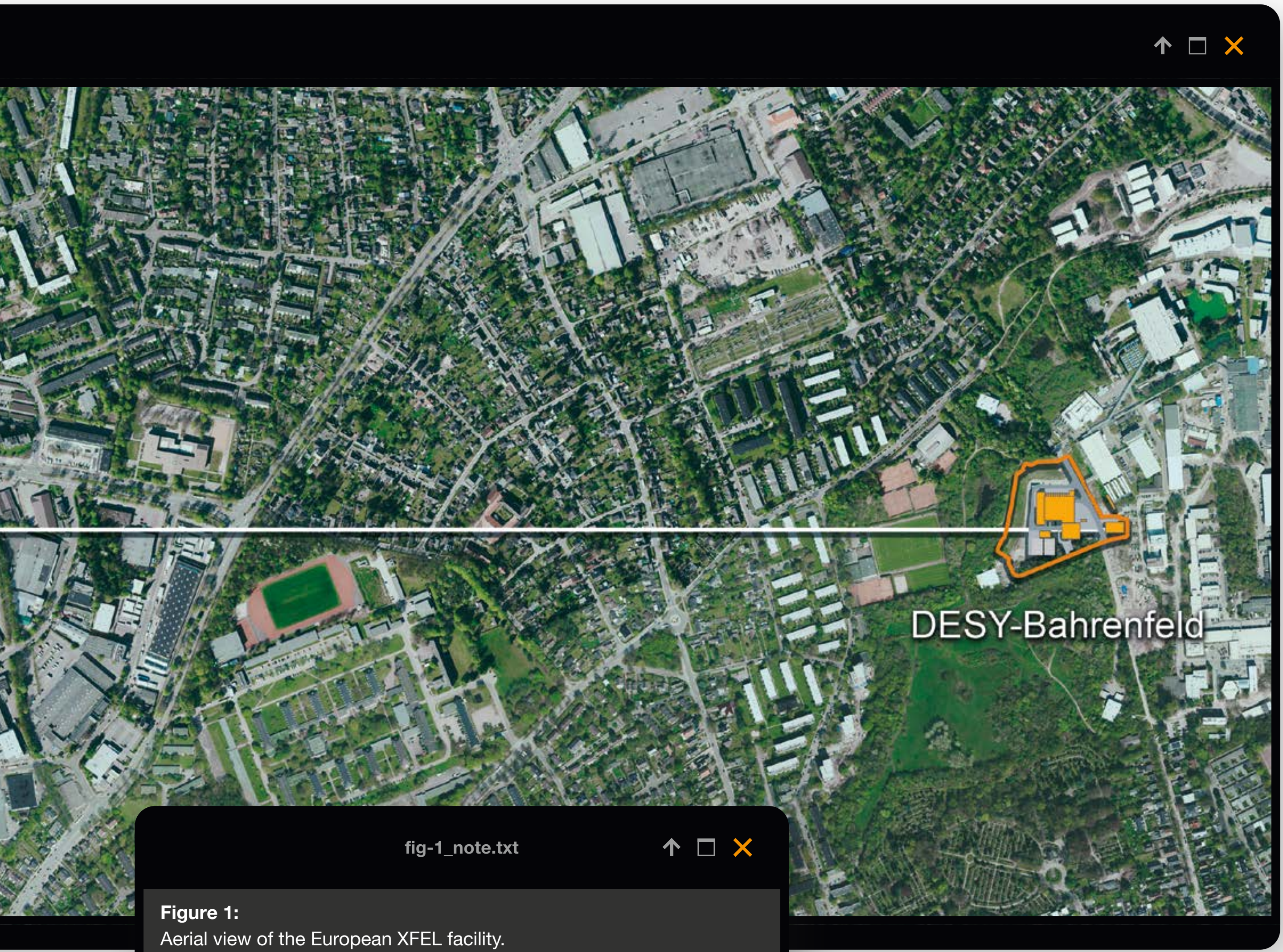


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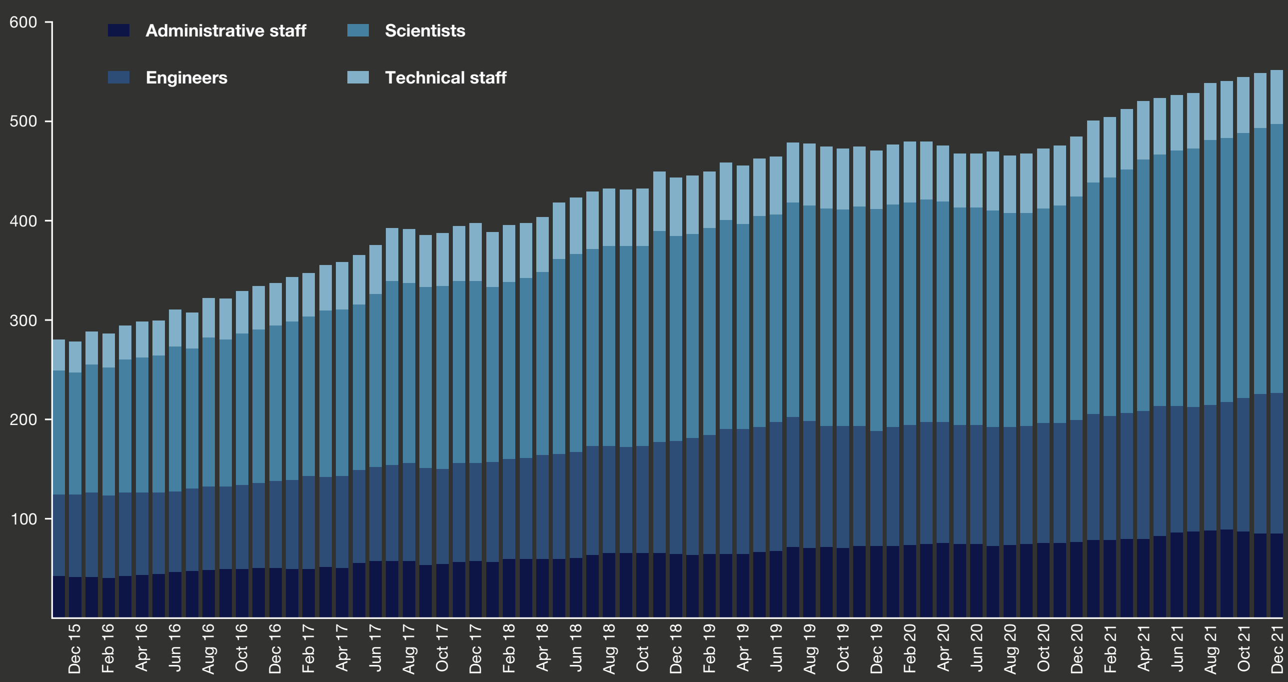
Figure 1:
Aerial view of the European XFEL facility.
Left to right: Schenefeld, Osdorfer Born, and DESY-Bahrenfeld sites.

Staff (1/2)

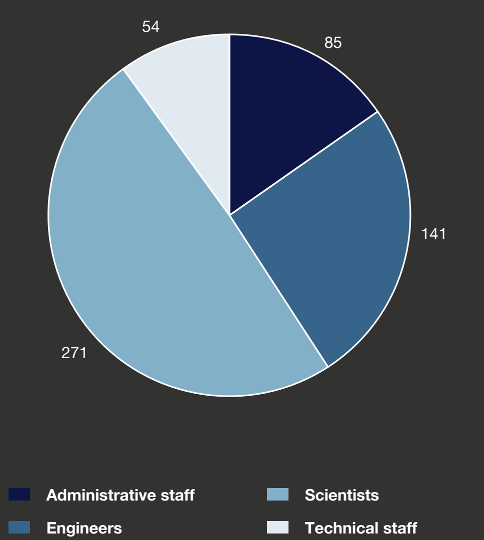
European XFEL employs staff members from 63 countries, bringing together various kinds of expertise to enable and support excellent and unique scientific research opportunities.

Staff development

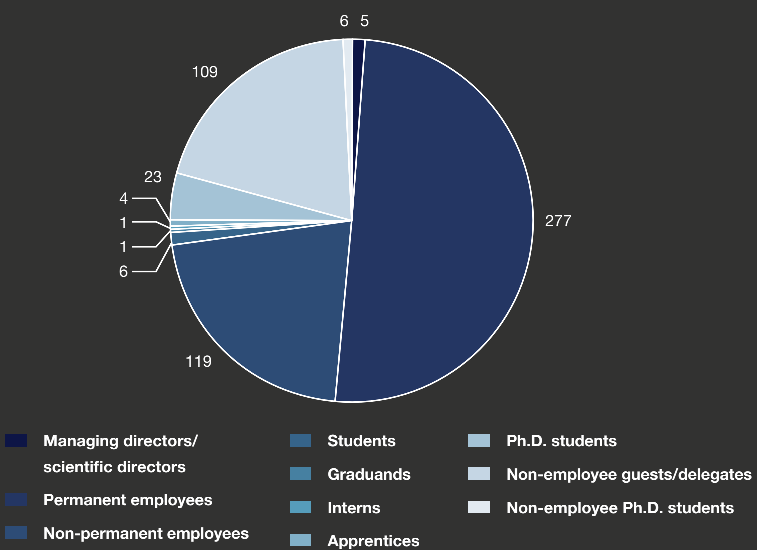
551 Total headcount including guests and completed contracts



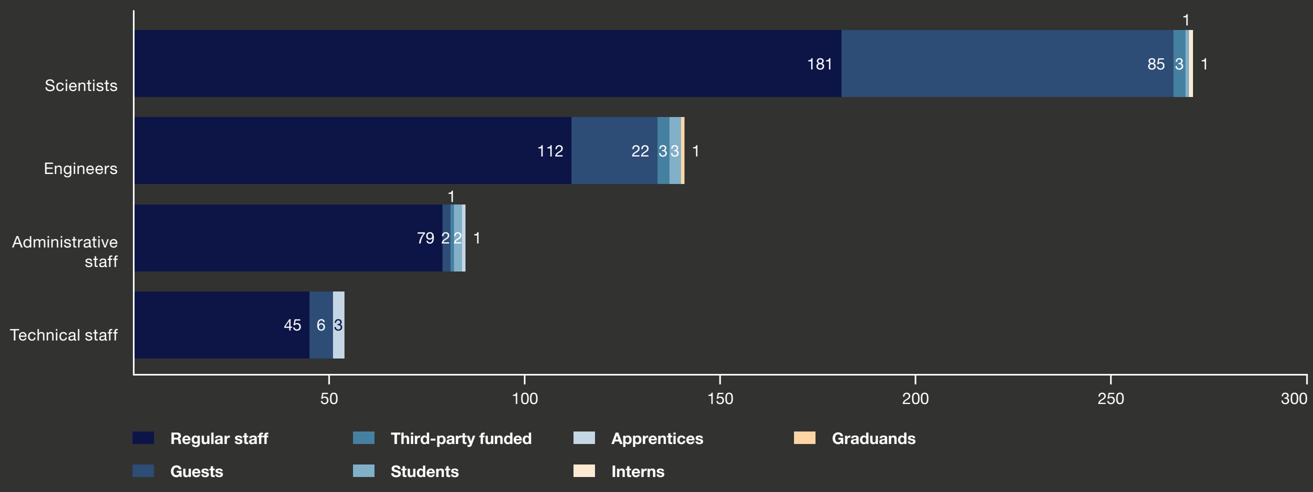
Functions



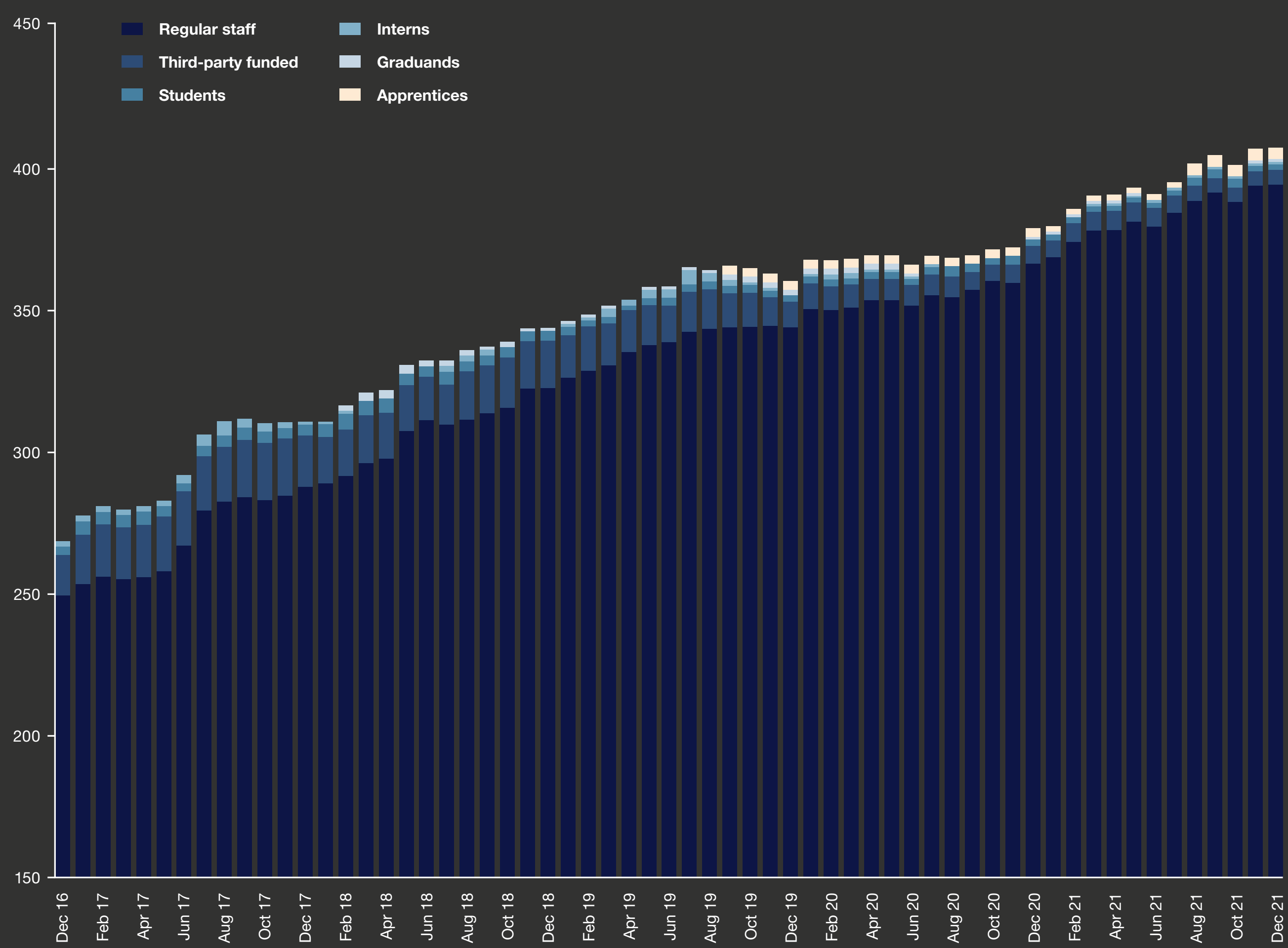
Contractual status



Function and contract split



Full-time equivalents | 406.78 Only actual European XFEL contracts

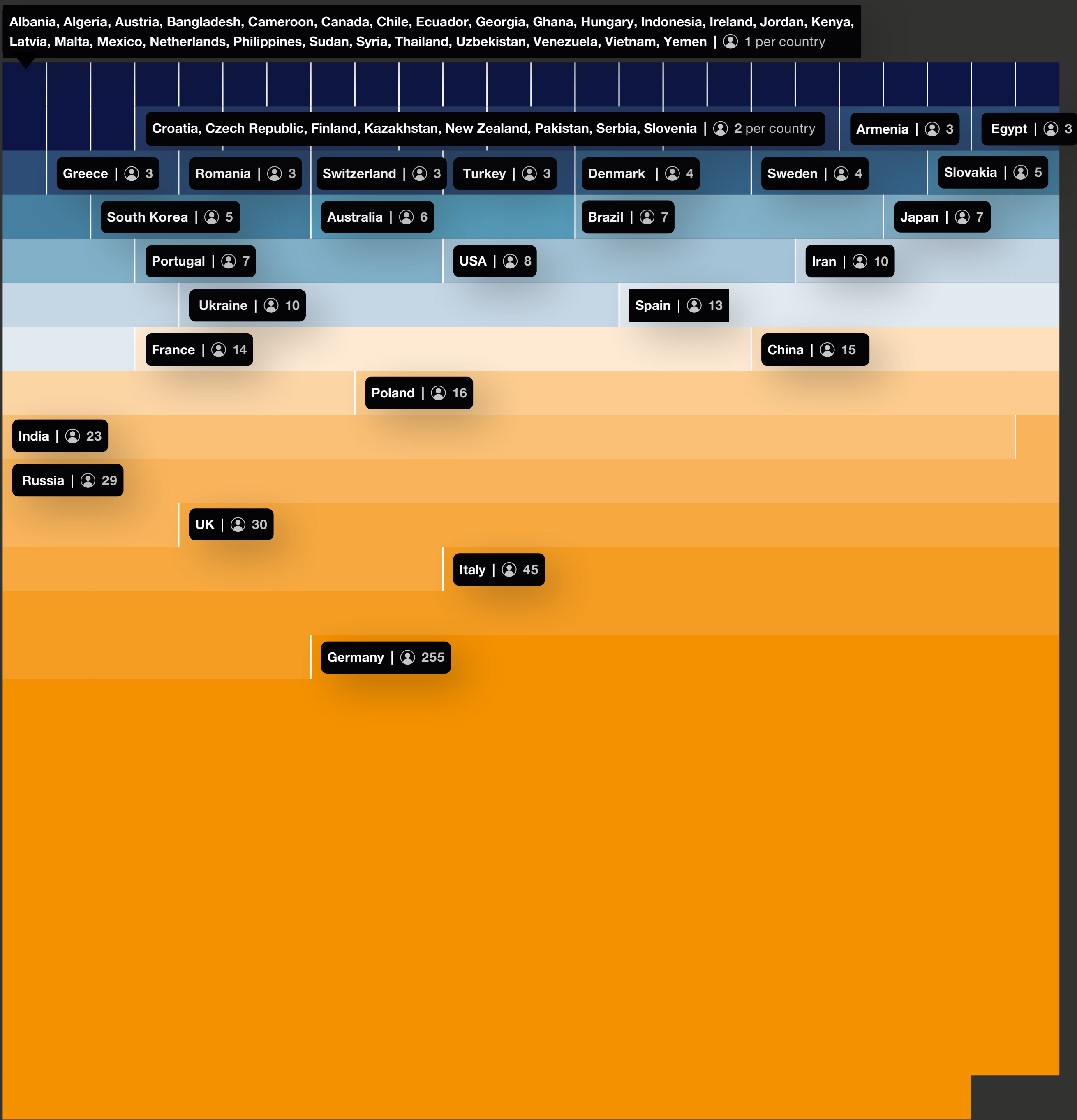


Staff (2/2)

All staff

63 Citizenships in total

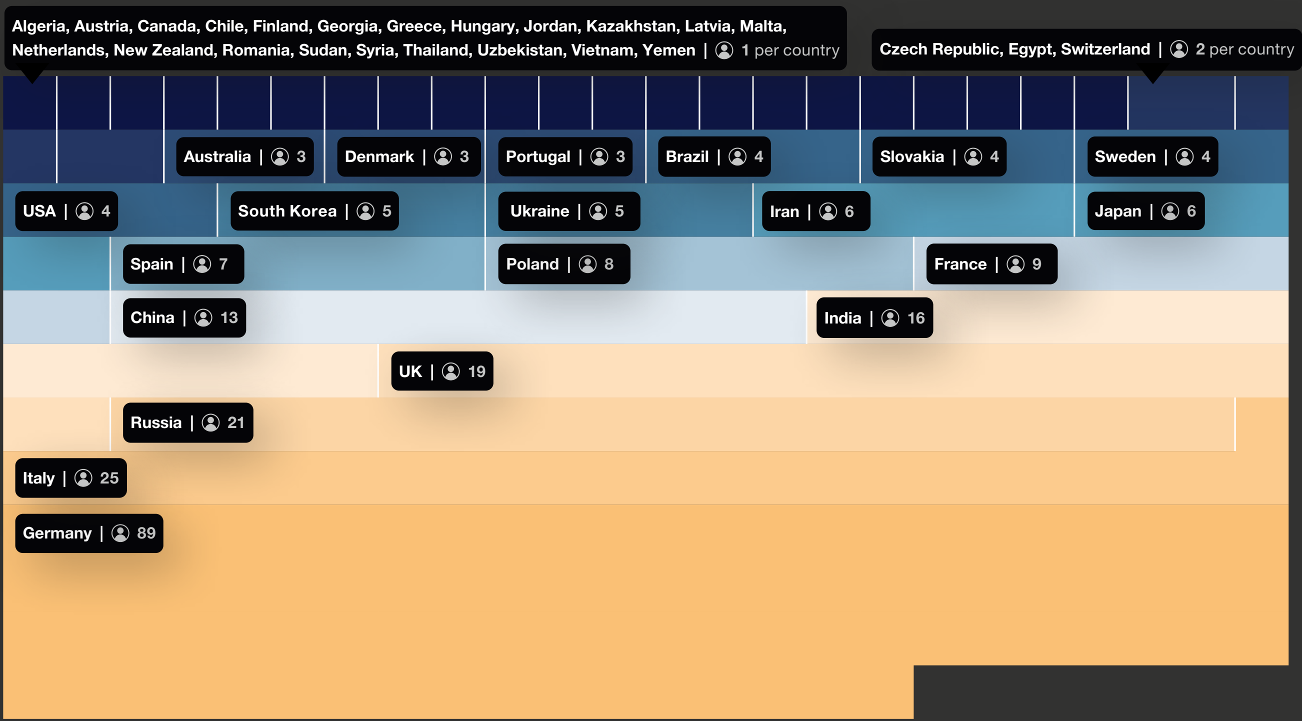
23 Double citizenships



Scientific staff

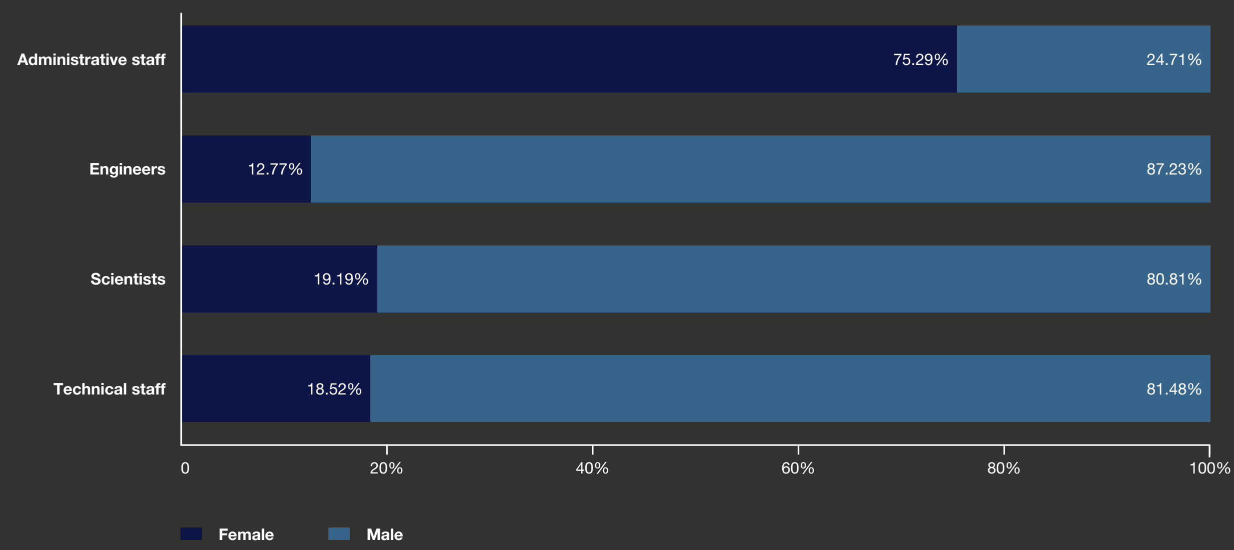
45 Citizenships in total

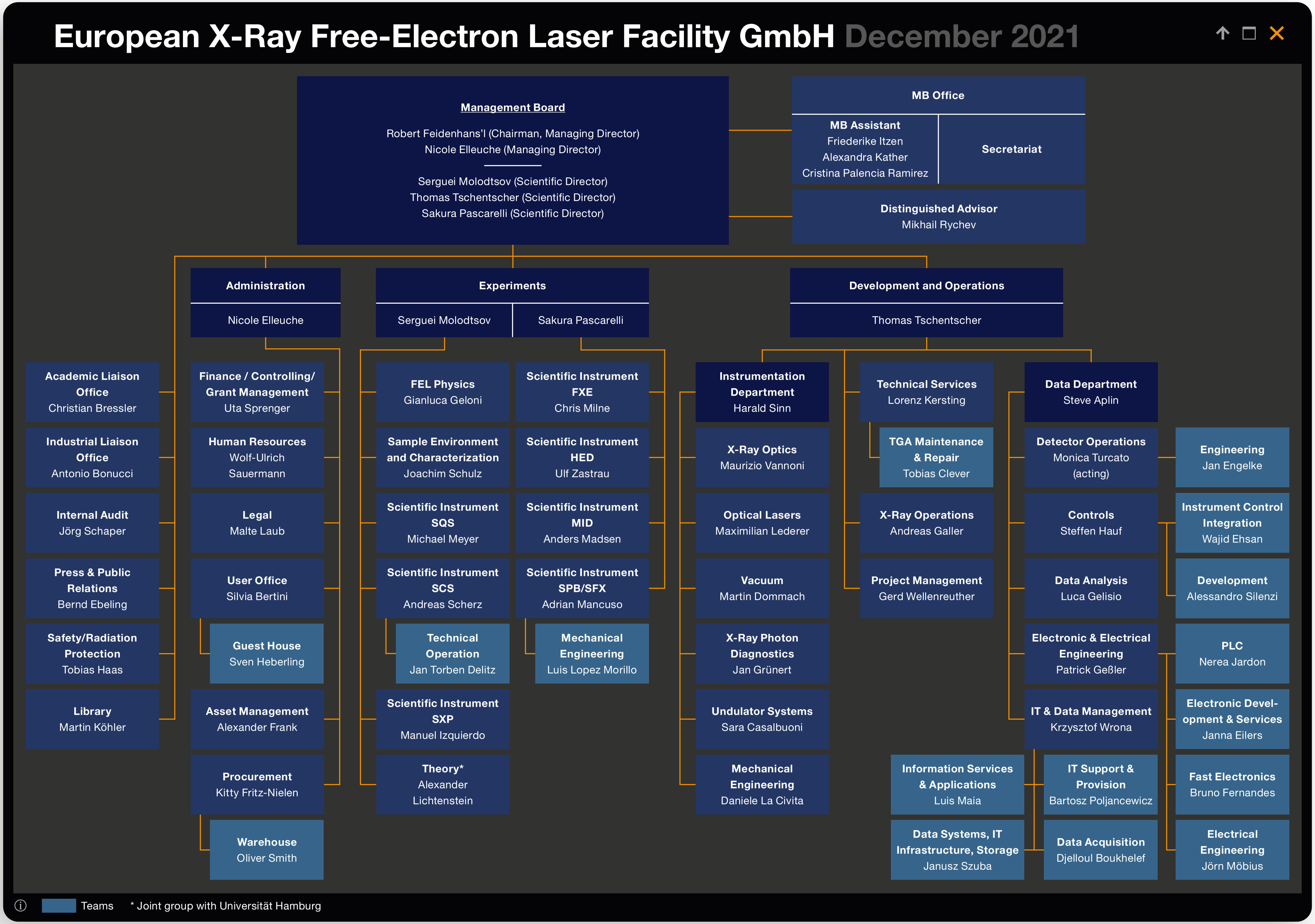
10 Double citizenships



Gender ratio

Total share of women **26.13%**




European X-Ray Free-Electron Laser Facility GmbH December 2021
Management Board
Robert Feidenhans'l (Chairman, Managing Director)
Nicole Elleuche (Managing Director)
Serguei Molodtsov (Scientific Director)
Thomas Tschentscher (Scientific Director)
Sakura Pascarelli (Scientific Director)
MB Office
MB Assistant Friederike Itzen Alexandra Kather Cristina Palencia Ramirez
Secretariat
Distinguished Advisor Mikhail Rychev
Administration Nicole Elleuche
Experiments Serguei Molodtsov Sakura Pascarelli
Development and Operations Thomas Tschentscher
Academic Liaison Office Christian Bressler
Industrial Liaison Office Antonio Bonucci
Internal Audit Jörg Schaper
Press & Public Relations Bernd Ebeling
Safety/Radiation Protection Tobias Haas
Library Martin Köhler
Finance / Controlling/ Grant Management Uta Sprenger
Human Resources Wolf-Ulrich Sauermann
Legal Malte Laub
User Office Silvia Bertini
Guest House Sven Heberling
Asset Management Alexander Frank
Procurement Kitty Fritz-Nielen
Warehouse Oliver Smith
FEL Physics Gianluca Geloni
Sample Environment and Characterization Joachim Schulz
Scientific Instrument SQS Michael Meyer
Scientific Instrument SCS Andreas Scherz
Technical Operation Jan Torben Delitz
Scientific Instrument SXP Manuel Izquierdo
Theory* Alexander Lichtenstein
Scientific Instrument FXE Chris Milne
Scientific Instrument HED Ulf Zastrau
Scientific Instrument MID Anders Madsen
Scientific Instrument SPB/SFX Adrian Mancuso
Mechanical Engineering Luis Lopez Morillo
Instrumentation Department Harald Sinn
X-Ray Optics Maurizio Vannoni
Optical Lasers Maximilian Lederer
Vacuum Martin Dommach
X-Ray Photon Diagnostics Jan Grünert
Undulator Systems Sara Casalbuoni
Mechanical Engineering Daniele La Civita
Technical Services Lorenz Kersting
TGA Maintenance & Repair Tobias Clever
X-Ray Operations Andreas Galler
Project Management Gerd Wellenreuther
Data Department Steve Aplin
Detector Operations Monica Turcato (acting)
Controls Steffen Hauf
Data Analysis Luca Gelisio
Electronic & Electrical Engineering Patrick Geßler
IT & Data Management Krzysztof Wrona
Information Services & Applications Luis Maia
Data Systems, IT Infrastructure, Storage Janusz Szuba
IT Support & Provision Bartosz Poljancewicz
Data Acquisition Djelloul Boukhelef
Engineering Jan Engelke
Instrument Control Integration Wajid Ehsan
Development Alessandro Silenzi
PLC Nerea Jardon
Electronic Devel-opment & Services Janna Eilers
Fast Electronics Bruno Fernandes
Electrical Engineering Jörn Möbius
Teams
* Joint group with Universität Hamburg

Shareholders

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

Member states	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** (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)

* Likely shareholder

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.

Chairwoman

Maria Faury (CEA, Paris)

Vice Chairman

Martin Meedom Nielsen (DTU, Kongens Lyngby)

Delegates

Denmark	**Morten Scharff** (DAFHES, Copenhagen)
France	**Sylvain Ravy** (CNRS, Paris)
	Patricia Roussel-Chomaz (CEA, Paris)
Germany	**Volkmar Dietz** (BMBF, Bonn)
	Helmut Dosch (DESY, Hamburg)
Hungary	**Györgyi Juhász** (NRDI 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** (Chalmers University of Technology, Gothenburg)
	Johan Holmberg (VR, Stockholm)
Switzerland	**Gabriel Aeppli** (PSI, Villigen)
	Laurent Salzarulo (State Secretariat for Education, Research and Innovation, Bern)
United Kingdom	**Helen Beadman** (UKRI, Swindon)
	James Naismith (Rosalind Franklin Institute, Didcot)

Observers

Spain	**Guadalupe C. de Córdoba Lasunción** (Ministerio de Ciencia e Innovación, Madrid)
	Rodolfo Miranda, since 8 June 2021 (IMDEA Nanociencia / Universidad Autónoma de Madrid)

Secretary

Malte Laub (European XFEL, Schenefeld)

Vice Secretary

Friederike Itzen (European XFEL, Schenefeld)

Next page: Advisers

European XFEL Council cont.

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Advisers

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

Previous page: Chairwoman, Vice Chairman, Delegates, Observers, Secretary, and Vice Secretary

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.

Chairman and Managing Director

Robert Feidenhans'l

Managing and Administrative Director

Nicole Elleuche

Scientific Directors and Proxy Holders

Serguei Molodtsov

Sakura Pascarelli

Thomas Tschentscher

Administrative and Finance Committee

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

Chairwoman

Sabine Carl (BMBF, Bonn, Germany)

Vice Chairman

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 (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	**Johan Holmberg** (VR, Stockholm)
Switzerland	**Peter Allenspach** (PSI, Villigen)
	Doris Wohlfender-Bühler (State Secretariat for Education, Research and Innovation, Bern)
United Kingdom	**Rachel Reynolds** (STFC, Swindon)

Secretary

Uta Sprenger (European XFEL, Schenefeld)

Vice Secretary

Deike Pahl (European XFEL, Schenefeld)

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.

Chairman

Andrzej Wolski, until 24 October 2021 (University of Liverpool, UK)
Evgeny Levichev, from 24 October 2021 (BINP, Novosibirsk, Russia)

Members

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

Chairman

Ian Robinson, until 20 November 2021 (UCL, London, UK)
Claudio Masciovecchio, from 21 November 2021 (Elettra Sincrotrone Trieste, Italy)

Members

Olga Alekseeva (IC RAS, Moscow, Russia)
Stefan Eisebitt, until 23 October 2021 (MBI, Berlin, Germany)
Guillaume Fiquet (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)
Jan Luening, from 18 November 2021 (HZB, Germany)
Claudio Maschiovecchio (Elettra Sincrotrone Trieste, Italy)
Keith Nugent, until 23 October 2021 (The Australian National University, Australia)
Arwen Pearson (Universität Hamburg, Germany)
Alexander Popov (ESRF, Grenoble, France)
Christoph Quitmann, until 23 October 2021 (RI Research Instruments GmbH, Bergisch Gladbach, Germany)
Philippe Wernet (Uppsala University, Sweden)
Robert W. Schoenlein (SLAC, Menlo Park, California, USA)
Nina Rohringer (DESY, Hamburg, Germany)
Ian Robinson (UCL, London, UK)
Tim Salditt, from 18 November 2021 (Georg-August-Universität Göttingen, Germany)

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)
Kay Rehlich (DESY, Hamburg, 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 involved in the development activities.

Chairman

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)

Secretaries

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

Proposal Review Panels

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

FXE Proposal Review Panel

Chairman

Michael Wulff (ESRF, Grenoble, France)

Vice Chairman

Wojciech Gawelda (Universidad Autónoma de Madrid, Spain)

Members

Shin-ichi Adachi (KEK, Tsukuba, Japan)
Federico Boscherini (University of Bologna, Italy)
Frank de Groot (Utrecht University, The Netherlands)
Thomas Elsässer (MBI, Berlin, Germany)
James McCusker (Michigan State University, East Lansing, Michigan, USA)
Alexander Soldatov (Southern Federal University, Rostov-on-Don, Russia)
Julia Weinstein (University of Sheffield, UK)
Philippe Wernet (Uppsala University, Sweden)

HED Proposal Review Panel

Chairman

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

Vice Chairman

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

Members

Michael Armstrong (LLNL, Livermore, California, USA)
Alessandra Benuzzi (LULI, Palaiseau, France)
Guillaume Fiquet (IMPMC, Paris, France)
Zahirul Islam (ANL, Lemont, Illinois, USA)
Stuart Mangles (Imperial College London, UK)
Mattias Marklund (Chalmers University, Gothenburg, Sweden)
Paul Neumayer (GSI, Darmstadt, Germany)
Norimasa Ozaki (Osaka University, Japan)
Sergey Pikuz (Joint Institute for High Temperatures, Moscow, Russia)

Next page: MID, and SCS Proposal Review Panels

Proposal Review Panels cont.

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MID Proposal Review Panel

Chairman

Giulio Monaco (University of Padova, Italy)

Vice Chairman

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

Members

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

SCS Proposal Review Panel

Chairman

Jan Lüning (HZB, Berlin, Germany)

Vice Chairman

Claudio Masciovecchio (Elettra Sincrotrone Trieste, Italy)

Members

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

Previous page: FXE, and HED Proposal Review Panels
Next page: SPB/SFX, and SQS Proposal Review Panels

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Proposal Review Panels cont.

SPB/SFX Proposal Review Panel

Chairwoman

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

Vice Chairman

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

Members

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

SQS Proposal Review Panel

Chairman

Eckhardt Rühl (Freie Universität Berlin, Germany)

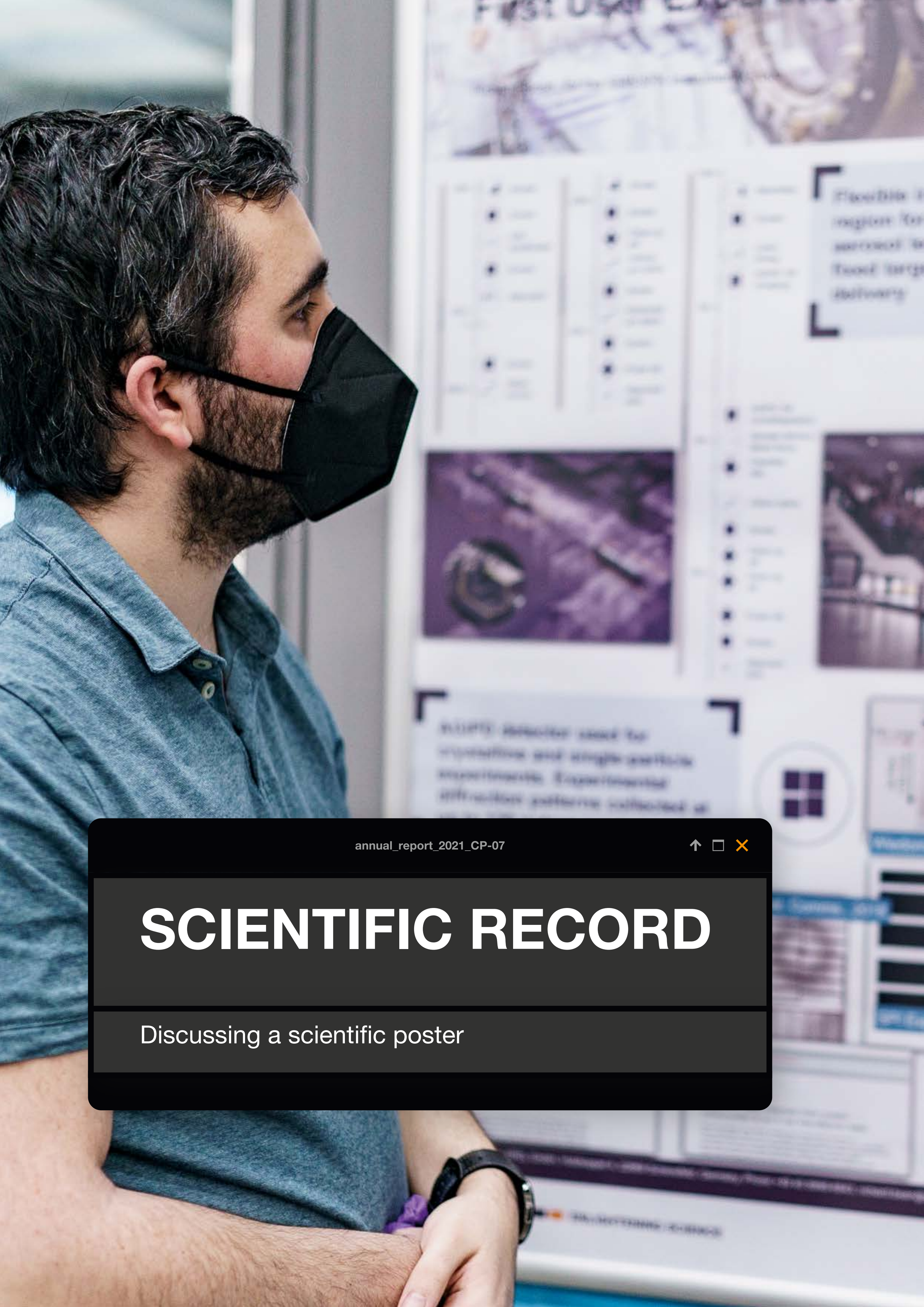
Vice Chairman

John Costello (Dublin City University, Ireland)

Members

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

Previous page: MID, and SCS Proposal Review Panels



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SCIENTIFIC RECORD

Discussing a scientific poster


Micron mirrors
installed, focus
max 3um (Nov 18)

Publications

User Publications

3D diffractive imaging of nanoparticle ensembles using an x-ray laser
K. Ayyer et al.: Optica **8** (1), 15 (2021)
doi:10.1364/OPTICA.410851

Analysis Strategies for MHz XPCS at the European XFEL
F. Dallari et al.: Appl. Sci. **11** (17), 8037 (2021)
doi:10.3390/app11178037

Data reduction for serial crystallography using a robust peak finder
M. Hadian-Jazi et al.: J. Appl. Crystallogr. **54** (5), 1360–1378 (2021)
doi:10.1107/S1600576721007317

Demonstration of an x-ray Raman spectroscopy setup to study warm dense carbon at the high energy density instrument of European XFEL
K. Voigt et al.: Phys. Plasma **28** (8), 082701 (2021)
doi:10.1063/5.0048150

High spatial coherence and short pulse duration revealed by the Hanbury Brown and Twiss interferometry at the European XFEL
R. Khubbutdinov et al.: Struct. Dyn. **8** (4), 044305 (2021)
doi:10.1063/4.0000127

High-resolution inelastic x-ray scattering at the high energy density scientific instrument at the European X-Ray Free-Electron Laser
L. Wollenweber et al.: Rev. Sci. Instrum. **92** (1), 013101 (2021)
doi:10.1063/5.0022886

Inner-Shell-Ionization-Induced Femtosecond Structural Dynamics of Water Molecules Imaged at an X-Ray Free-Electron Laser
T. Jahnke et al.: Phys. Rev. X **11** (4), 041044 (2021)
doi:10.1103/PhysRevX.11.041044

Microsecond hydrodynamic interactions in dense colloidal dispersions probed at the European XFEL
F. Dallari et al.: IUCrJ **8** (5), 775–783 (2021)
doi:10.1107/S2052252521006333

Nanosecond timing and synchronization scheme for holographic pump–probe studies at the MID instrument at European XFEL
M. Osterhoff et al.: J. Synchrotron Radiat. **28** (3), 987–994 (2021)
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Workshops and Seminars

20–29 JANUARY 2021
European XFEL Users' Meeting
Virtual event

The European XFEL Users' Meeting is an annual opportunity to strengthen the interaction between European XFEL and the scientific user community. Due to the restrictions in place during the COVID-19 pandemic, the 2021 Users' Meeting and the satellite meetings were organized as virtual events. Nevertheless, the joint organization with DESY Photon Science and the format of the meeting could be maintained, including topical satellite meetings and (online) poster sessions. About 2000 scientists registered for events, representing 40 countries and all of the European XFEL partners.

The scope of the plenary meeting included updates on the progress and current status of the European XFEL, scientific highlights from all six scientific instruments with presentations by facility users, including the first European XFEL Young Scientist Award winner. Members of the User Organization chaired the plenary sessions, gave an activity report, and presented the results of the first user survey they had organized. The online satellite meetings addressed different topics: the HED instrument and the HiBEF User Consortium, the FXE instrument, data user experience, and the automated high-repetition-rate sample delivery for single-shot experiments.

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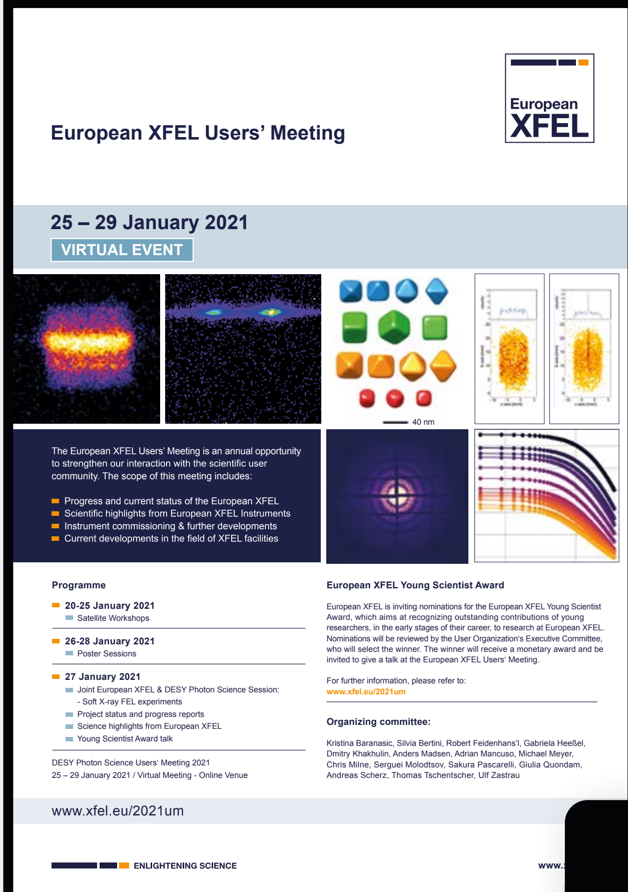

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fig-1

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Figure 1:
European XFEL Users' Meeting announcement poster (left) and Michael Schneider (upper right), recipient of the first European XFEL Young Scientist Award (bottom right)

Workshops

21 JANUARY 2021 – 24 NOVEMBER 2022
Virtual Hard X-Ray Collaboration Seminar Series
The Virtual Hard X-Ray Collaboration Seminar Series hosts 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 are spread throughout 2021 and 2022, with lecturers from Germany, the USA, Switzerland, Korea, Japan, and China taking turns presenting topics and chairing the meetings.

18 FEBRUARY 2021
Big Science Business Forum Webinar
This webinar introduced technology transfer in big science and how to improve it from academic and scientific institutions to industry. It also provided an interview and tour of big science organizations (FELs OF EUROPE, CERN, ESA, EMBL) and technology transfer technology.

1 MARCH 2021 – 4 APRIL 2022
FELs OF EUROPE Tutorials
Science@FELs 2020, the first online Science@FELs conference, 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.

1 MARCH 2021
FELs OF EUROPE Tutorial: FEL Basics, Generation, and Applications
This tutorial aimed to explain the simple physics behind FELs, with an elementary introduction to synchrotron radiation, including properties such as the emitted wavelengths, flux, angular collimation, brightness, and coherence. It also introduced the FEL mechanism—explaining fundamental properties such as bunching, coordinated emission, and time structure—as well as some FEL applications, such as femtosecond experiments and new techniques based on fundamental quantum properties.

24–26 MARCH 2021
Opportunities and Challenges of Cavity-Based X-Ray Free-Electron Lasers
This workshop summarized the various concepts for cavity-based X-ray FELs and related schemes, including projected X-ray radiation performance parameters for the respective schemes; described initial concepts for accelerator, X-ray optics, and other X-ray instrumentation systems; identified the most important performance requirements for each critical subsystem; and identified promising X-ray techniques and scientific opportunities for strong science cases.

19–21 APRIL 2021
Virtual Superconducting Undulators for Advanced Light Sources
This workshop summarized the parameters for applications at X-ray FELs and diffraction-limited storage rings; described requirements for plasma-based accelerators; identified the requirements and challenges of different magnetic geometries for helical superconducting undulators; and identified existing technologies and R&D for current projects as well as potential technologies and R&D for future projects.

2–3 JUNE 2021
Fluctuation X-Ray Scattering
This workshop reviewed recent theoretical and methodological advances in fluctuation X-ray scattering (FXS) as well as applications of the FXS approaches for materials research at storage rings, FELs, and other facilities.

8 JUNE 2021
Artificial Intelligence Workshop at EuXFEL
This online workshop was hosted by European XFEL to discuss the latest developments in artificial intelligence as applied to photon science.

14–18 JUNE 2021
Ultrafast X-Ray Summer School (UXSS) 2021
The summer school was virtually hosted by CFEL at DESY, and jointly organized by CFEL and the PULSE institute at SLAC. The summer school programme was highly interdisciplinary, with topics ranging from accelerator physics to molecular biology, and was intended to give doctoral students and postdoc researchers the opportunity to familiarize themselves with the latest developments and opportunities in ultrafast X-ray science.

22–24 JUNE 2021
Third Workshop on Scientific Archives
This workshop was virtually hosted by European XFEL. International speakers discussed topics about scientific archives, records, and data.

28–30 JUNE 2021
Attosecond to Few-Femtosecond Ultrafast Science at Future FELs
This workshop described the visions of key ultrafast science questions 5–10+ years from now; major drivers in different fields, from atomic, molecular, and optical physics as well as non-linear physics through chemistry to condensed-phase and (quantum-)materials science; and accelerator/undulator concepts necessary for the envisaged science. It also attempted to stimulate thinking “outside the box” about currently ongoing or near-future activities.

29 SEPTEMBER 2021
Development in Undulator Technology
This workshop focused on the implementation of new strategies and activities for long-term partnerships between industry and the European light sources, synchrotrons, and FELs, with their tens of thousands of users, in order to strengthen highly specialized European companies for the light source market worldwide.

6 OCTOBER, 11 NOVEMBER, and 30 NOVEMBER 2021
Big Science Business Forum Webinar Miniseries
These webinars identified the technologies that will drive future projects, investigating strategies for the future and related R&D programmes as well as how industry can get involved.

21–22 OCTOBER 2021
Workshop on 1D Imaging Soft X-Ray Spectroscopy at the SQS Instrument of the EuXFEL
This workshop discussed the scientific opportunities offered by the installation of a 1D imaging soft X-ray spectrometer at the European XFEL SQS instrument.

2–3 NOVEMBER 2021
Science Opportunities in Condensed-Phase Chemistry with Femtosecond Hard X-Ray Methods
This workshop included presentations by X-ray FEL facility representatives, with an overview of the way researchers are using hard X-ray instruments to answer chemical, materials, or biochemical questions with hard X-ray probes. It also included presentations by X-ray FEL management representatives, with an overview of how facilities have encouraged chemical research using the various tools available to provide beam access (long-term proposals, standard configurations, scientific campaign proposals, etc.). Finally, it provided research seminars from experienced researchers who have used a variety of X-ray FEL facilities for their research as well seminars on potential future areas of X-ray FEL science.

Seminars

THEORY SEMINARS

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

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

10 JUNE
Vibrational spectroscopy and dynamics of the hydrated proton by full-dimensional quantum mechanics
Oriol Vendrell, Heidelberg University (Germany)

17 JUNE
Photodissociation of ironpentacarbonyl $Fe(CO)_5$—from initial bursts of CO release to branching pathways in solution
Michael Odelius, Stockholm University (Sweden)

24 JUNE
Modeling of ultrafast X-ray induced demagnetization in magnetic multilayer systems
Victor Tkachenko, IFJ PAN (Poland) and European XFEL (Germany)

8 JULY
The curious case of superconducting infinite-layer nickelates
Frank Lechermann, European XFEL (Germany) and Flatiron Institute (USA)

30 SEPTEMBER
Development of free-energy density functional methods for warm dense matter applications
Valentin V. Karasiev, Laboratory for Laser Energetics, University of Rochester (USA)

7 OCTOBER
Strong suppression of heat conduction in laboratory and astrophysical plasmas
Gianluca Gregori, Oxford University (UK)

11 NOVEMBER
X-ray spectroscopy studies of molecules and materials with TDDFT-based approaches: recent applications and developments
Niri Govind, Pacific Northwest National Laboratory (USA)

18 NOVEMBER
Structure and damage of disordered materials: opportunities for XFEL science
Andrew Martin, RMIT University (Australia)

SCIENCE SEMINARS

19 JANUARY
Measuring photo-induced dynamics in the attosecond time domain
Jon Marangos, Blackett Laboratory Extreme Light Consortium, Imperial College London (UK)

2 FEBRUARY
X-ray imaging at the nanoscale with attosecond temporal resolution
Tais Gorkhover, Universität Hamburg (Germany)

16 FEBRUARY
Real-time observation of conical intersection in biomolecules
Giulio Cerullo, Politecnico di Milano (Italy)

2 MARCH
Mechanistic insight into vitamin B12 chemistry: femtosecond X-ray spectroscopy of cobalamins
James Penner-Hahn, Departments of Chemistry and Biophysics, University of Michigan (USA)

16 MARCH
Non-thermal photo-induced metallic phase emerging from nanoscale complexity in correlated quantum materials
Claudio Giannetti, Department of Mathematics and Physics, Università Cattolica del Sacro Cuore (Italy)

30 MARCH
Attosecond charge migration in bio-relevant molecules: controlling the photochemistry at the electron time scale
Francesca Calegari, Attosecond Science Group, CFEL, DESY (Germany)

13 APRIL
Recent advances in probing excited states of solids by time-resolved ARPES
Martin Wolf, Fritz Haber Institute, Physical Chemistry, Max Planck Society (Germany)

27 APRIL
LCLS today & tomorrow: recent science, future opportunities & development plans
Robert Schoenlein, Linac Coherent Light Source, SLAC National Accelerator Laboratory (USA)

11 MAY
Theory of collective spontaneous X-ray emission
Nina Rohringer, DASHH Spokesperson, DESY (Germany)

25 MAY
Time-resolved photoelectron spectroscopy @ EU-XFEL: ideas and challenges from soft to hard X-ray
Giancarlo Panaccione, IOM, CNR National Research Council (Italy)

6 JULY
Polaritonic quantum materials from first principles
Angel Rubio, CFEL / Max Planck Institute for the Structure and Dynamics of Matter (Germany)

21 SEPTEMBER
A hard X-ray diffraction microscope at an XFEL: a new paradigm for bulk materials
Henning Friis Poulsen, Dept. of Physics Neutrons and X-rays for Materials Physics, Technical University of Denmark

19 OCTOBER
Quantifying the dose absorbed by samples in XFEL experiments: an aid to determining radiation damage free structures
Elspeth Garman, Dept. of Biochemistry, University of Oxford (UK)

16 NOVEMBER
X-ray lasers for chemical and bio-inorganic spectroscopy
Philippe Wernet, Chemical and Bio-Molecular Physics Program, Dept. of Physics and Astronomy, Uppsala University (Sweden)

30 NOVEMBER
A perspective on some future directions for dynamic compression experiments at XFEL
Justin Wark, University of Oxford (UK)

21 DECEMBER
Shifting time-resolved structural biology from a niche pursuit to a standard experiment
Arwen Pearson, The Hamburg Centre for Ultrafast Imaging (Germany)

Lecture series

27 SEPTEMBER – 1 OCTOBER
Lecture series "Materials Research with Free-Electron X-Ray Lasers"
The lecture series is jointly organized by European XFEL and Technische Universität Bergakademie Freiberg and was held online in 2021. The students gain a deeper knowledge of the structure and use of X-ray free-electron lasers (FELs). Topics include inelastic and resonant inelastic X-ray scattering (IXS and RIXS), X-ray emission spectroscopy (XES), X-ray absorption spectroscopy (XAS), photoelectron spectroscopy (XPS and ARPES), X-ray microscopy, coherent X-ray diffraction (CDI), photon correlation spectroscopy (PCS), and X-ray holography. A virtual excursion was also part of the lecture series.

Glossary

A

AGIPD
Adaptive Gain Integrating Pixel Detector
[European XFEL detector]

B

BAM
beam arrival time monitor

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

DAC
diamond anvil cell

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

DESY
Deutsches Elektronen-Synchrotron in Hamburg and Zeuthen, Germany

DFG
German Research Foundation

DOC
Data Operation Centre at the European XFEL

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

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

PAM
pulse arrival time monitor

PETRA III
Synchrotron radiation facility at DESY in Hamburg, Germany

PLC
programmable logic controller

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]

T

TGA
Technical Building Infrastructure at European XFEL

U

UKRI
UK Research and Innovation in Swindon, UK

V

VR
Swedish Research Council in Stockholm, Sweden

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