2019

10th Anniversary

## ANNUAL REPORT

Developments, Results, Impressions



### European XFEL Annual Report 2019

Construction	
Start of commissioning	
First user experiments	

Total length of the facility Total length of the tunnel system Depth of the tunnels

3.4 kilometres 5.8 kilometres 6 to 38 metres

2009 – 2017 2016 2017



Fig. 1

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01: Robert Feidenhans'l, 02: Nicole Elleuche, 03: Serguei Molodtsov, 04: Sakura Pascarelli, 05: Thomas Tschentscher IIN

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### MANAGEMENT BOARD FOREWORD

It is truly inspiring to walk through the experiment hall into the instrument control rooms when our users are on the campus, watch the first experiment results show up on the screens, and discuss them with the users. The place is buzzing with enthusiasm and excitement.

In 2019, we saw the first visions come alive. Six instruments are now operational, enabling exciting science. Not that it has been plain sailing. It has taken a lot of hard work to make sure that users can carry out their ambitious experiments. At the end of our second full year of operation, we are very pleased to experience a much higher reliability of our optics, vacuum, controls, and diagnostic systems. The accelerator and the three SASE beamlines can simultaneously be tuned to achieve a variety of operating conditions, and we are now able to run three instruments in parallel. This is a unique feature, which allows us to host more scientists and experiments per unit of time than other X-ray FEL facilities.

We were also able to perform first in-house experiments at the design pulse repetition rate of 4.5 MHz and enable user experiments at a photon wavelength of 0.7 Å. Five peer-reviewed journal articles published by our users in 2019 showcase the potential of the facility. None of these developmental and technical milestones would have been possible without the close and effective collaboration of scientists and engineers across European XFEL and at our partner, DESY.

Our ventures into new terrain are enabled through the continued support and trust of our shareholders. We are extremely thankful that the European XFEL Council agreed to our request to increase the operating budget. These extra funds ensure that we can further develop our instruments and have the human resources to maintain and run them for our users.

In 2019, as we moved toward full user operation, we initiated several organizational changes within the company. These changes aim to improve the communication between groups, provide a more effective distribution of resources, and streamline processes to make work more efficient and workloads more sustainable. Change is never easy, and we are thankful for the trust our staff has shown in us over the past year. We think everyone is now starting to see the benefits of these changes. One of the most visible internal reorganizational changes has been the establishment of the new Development and Opera-

tions Division, which encompasses the Instrumentation and Data Departments, the X-Ray Operations group, the Project Management Office, and Technical Services.

In September, Sakura Pascarelli from ESRF joined us as scientific director on the management board. We are very pleased to have her on board. Sakura oversees the further development of the hard X-ray instruments as well as the in-house research and our Ph.D. student programme.

On our research campus in Schenefeld, the opening of our company restaurant, BeamStop, which offers tasty meals to staff members, visiting scientists, and local residents, has been a huge cultural shift for everyone on site.

In this annual report, we present the highlights and successes of the last 12 months. In Chapter 3, we look back at the eventful 10-year history of our facility. With all scientific instruments operational and first results published, the founding date of European XFEL and the start of construction in 2009 seem to belong to a distant past. This is reflected in the layout and design of this annual report, which we hope you will enjoy reading.

Finally, we would like to thank you for your continued support, trust, and input. European XFEL is a unique and complex facility, and we greatly value the diversity and richness of perspectives and experiences that everyone contributes, ensuring that European XFEL remains innovative and creative along our journey to discoveries that have a significant and valuable impact on science and society.

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Robert Feidenhans'l

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Maria Faury - Chairperson of the European XFEL Council

### **COUNCIL CHAIR FOREWORD**

Like previous years, 2019 was an intense year in many aspects. Among the highlights was the celebration of European XFEL's 10-year anniversary.

On 30 November 2009, representatives from 10 partner countries signed the European XFEL Convention and Final Act in the Hamburg city hall, thus establishing the European XFEL GmbH. The European XFEL member states joined forces to build and operate the world's largest X-ray laser facility, opening up completely new research opportunities for the scientific community. The promises have been kept, and the results are in line with our ambitious expectations.

The European XFEL facility has now been in operation for more than two years. In this time, it has grown in power, with all the instruments made available to the scientific community. Meanwhile, more than 80 user experiments have been performed and more than 1200 users have been welcomed on site, leading to an increasing number of publications of the European XFEL staff, the DESY accelerator staff, and the European XFEL Management Board.

I would like to take this opportunity to thank the European XFEL Council for its commitment, its trust, and its ongoing support. After a one-year scrutiny of budget figures by a dedicated working group, the council agreed to increase the operating budget of European XFEL for the coming years. This was an important decision made by the shareholders, who agreed to increase their own contributions in order to enable the further successful development of the company. The European XFEL is now definitively ready to enter its full operating regime.

On the management side, we had the pleasure of welcoming Sakura Pascarelli, who started as scientific director at European XFEL in September 2019. Reorganizations within the company have been implemented to ensure that tasks can be addressed in a most effective way.

The campus is developing nicely, and European XFEL has celebrated the opening of the company restaurant, the well-named "BeamStop". The next steps will be to build the guest house and the visitor centre.

Many exciting challenges are awaiting us in 2020: offering more beamtime with simultaneous access to the instruments, diversifying and expanding the user community, ensuring reliable operation, and preparing the transformation from share- to usage-based operation cost repartition in 2023.

I have full confidence in the European XFEL management and governance bodies to successfully achieve these objectives, as we are all truly committed to the success of this unique facility.

M. Fan

Maria Faury



# HIGHLIGHTS

### UNRAVELLING PHOTOCATALYTIC REACTIONS BY TWO COLOUR X-RAY EMISSION

Matthias Bauer, Paderborn University, Germany

Base metal photoactive compounds are sustainable alternatives to their noble-metal counterparts. Bimetallic assemblies of the latter are often used for direct conversion of sunlight into chemical energy carriers, such as hydrogen. The transition to base metal dyads as active compounds is partially hindered by the so-far missing deeper understanding of the working principle of such hetero-bimetallic complexes, which is required to improve their photocatalytic performance. Therefore, studies of the ultrafast photoinduced electron transfer are of utmost importance on the way to active base metal dyads for photocatalytic electron transfer reactions. In an experiment at the FXE instrument at the European XFEL, we used femtosecond ultrafast X-ray emission spectroscopy (XES) to track the electronic and structural dynamics in a bimetallic assembly, connecting an iron photosensitizer to a cobaloxime catalyst for photocatalytic proton reduction. Due to the intrinsically ultrafast nature of the investigated processes, partially unknown excited states at the iron photosensitizer, and optically dark states at the cobaloxime catalyst, the femtosecond two-colour XES experiment was applied for the first time, simultaneously detecting iron and cobalt K X-ray emission to avoid ambiguities about the time zero. In this way, it was possible to unequivocally correlate the ultrafast excited-state dynamics to electron transfer processes within the dyad.

The excited-state dynamics and photoinduced electron transfer from a photosensitizer to a catalyst are the initial processes that determine the working principle and activity of dyads in photocatalytic reduction reactions. Accordingly, the charge transfer originates from nonequilibrated states, and conventional analytic tools cannot be applied to understand its correlation to the chemical structure of the assembly. Ultrafast spectroscopy using optical lasers and, more recently, X-ray free-electron lasers (FELs) made the regime of such processes available. Upon photoexcitation, the subsequent excited-state dynamics in hetero-bimetallic dyads involve the population and relaxation of metal-to-ligand charge transfer (MLCT) states, ligand-to-metal charge transfer (LMCT) states, metal-centred (MC) states, and ligand-mediated metal-to-metal charge transfer (MMCT) states. Ultrafast XES is a powerful tool allowing these states and their relative contribution to the ongoing dynamics [1] to be identified and discriminated. In particular, for Fe–Co dyads (Figure 1), where the involved cobalt states are typically optically silent [2], two-colour XES is the only method enabling the excited-state dynamics at the iron photosensitizer to be linked to those at the cobaloxime catalyst.

In our two-colour XES experiment at the FXE instrument [3], we measured a simultaneous excitation of iron and cobalt with a time resolution of 140 fs [4]. Samples of the Fe-Co dyad, which were provided in solution by means of a liquid jet, were excited with an optical laser and probed by the X-ray beam. Data was collected in an energy-dispersive manner using a von Hamos XES spectrometer and a 2D charge-integrating Jungfrau detector (Figure 1a). As a reference for the dyad measurement, the cobalt part (the catalyst) and the iron part (the photosensitizer) were also measured in the same experimental conditions. For the initial data correction, the experiments were sorted, background-reduced, filtered, and normalized to obtain XES spectra as a function of the delay time between the optical pump pulse and the X-ray probe pulse. From that series of XES spectra, differential transient XES (ΔXES) spectra were calculated (Figure 1b, d). Progressive changes in the ΔXES profiles can be represented in the form of integrals of the selected feature over all delay times (Figure 1e). Those kinetics were subsequently fitted with fluorescence rise and multiexponential decay functions to obtain decay rates.

Short-time-scale kinetics for pure cobaloxime revealed only one decay time constant of 0.7 ps, while kinetics for the photosensitizer indicated three decay time constants in total: 9 ps, 1.7 ps, and ~0.2 ps. The shortest time constant in the photosensitizer could be assigned to either a contribution from vibrionic wave packet cooling



[5] or a short-lived <sup>1</sup>MLCT state [1]. The two longer time constants were tentatively assigned to a <sup>3</sup>MLCT state (9 ps) and a <sup>3</sup>MC state (1.7 ps), in agreement with the available literature [1]. When the iron photosensitizer was connected to the cobaloxime catalyst, forming a dyad, the iron-related decay constants changed to 10.4 ps, 1.7 ps, and ~0.2 ps, while the cobalt-related decay rates were significantly different from pure cobaloxime: 6 ps and ~0.2 ps (Figure 1e). Consequently, one of the ironrelated time constants was shorter than in the pure photosensitizer, while new and longer time constants were found at the cobalt emission in the dyad. In particular, we propose that the 6 ps time constant could be connected to a charge density change at the cobalt, resulting from an electron transfer from the iron centre (rather than a direct photoexcitation of the cobalt moiety). This preliminary conclusion has to be further corroborated in future experiments and by means of advanced theoretical

calculations.

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### MAKING MOLECULAR MOVIES AT THE EUROPEAN XFEL

Marius Schmidt, University of Wisconsin-Milwaukee, USA

The European XFEL is a 3.4 km long engineering marvel dedicated to producing the brightest X-rays in the world. With these X-rays, one can reach magnifications, or resolutions, high enough to see atoms. The European XFEL is so powerful that it can film how the atoms move around during a chemical reaction. Think of combustion: Molecules of oxygen and fuel are mixed. After ignition, the oxygen reacts with the fuel, and the molecules fly apart violently. Researchers want to film such processes in atomic detail, and this requires an enormous amount of X-ray light. It is even more complicated to follow the reactions of life. The European XFEL has been specifically designed to film biologically relevant reactions in extreme slow motion and with extreme resolution. In 2019, for the first time at the European XFEL, an international team of researchers produced such a molecular movie. We watched atomic motions in a protein called photoactive yellow protein (PYP) on ultrafast time scales. The success of this experiment has big implications on how to conduct experiments at the European XFEL.

All known life functions consist of chemical reactions. These reactions are facilitated by a large number of proteins. Although proteins are polymers, they display highly ordered shapes, or structures. There is a huge variety of proteins, each with a structure that promotes a specific function. When the first structure of a protein, that of myoglobin, was solved, researchers were already interested in details of its function. Myoglobin binds oxygen and is poisoned by carbon monoxide. These gas molecules can be detached from their binding site by a laser. Shortly afterwards, the molecules rebind. By filming the rebinding process, researchers are able to reveal the myoglobin's function. It took about 40 years of R&D until this was possible, using time-resolved crystallography at a synchrotron X-ray source. Although very short, the pulse duration of the X-ray flashes delivered by the synchrotron was still too long, however, to follow the fastest events of the reaction.

In 2009, the first X-ray free-electron laser (FEL), the Linac Coherent Light Source (LCLS) in the USA, came online. An X-ray FEL has a pulse duration that is more than a

thousand times shorter than at a synchrotron source, and the X-ray pulses are much brighter. They can be used to investigate samples that are so tiny they cannot be seen with the naked eye. However, there is a catch. X-rays are damaging-the X-rays from an X-ray FEL are so intense that the sample is destroyed. Fortunately, data are collected almost instantaneously, while the damage evolves more slowly, making it possible to take essentially damage-free pictures. To this end, fresh samples must be provided one by one, which can be achieved by embedding them in a fast-moving liquid jet that is exposed to the X-ray pulses. In the early experiments at LCLS, data quality was not that great, and the resolution was low. Scientists were sceptical about whether the data would ever be good enough to make a molecular movie. An international collaboration of scientists then managed to demonstrate how to collect a single snapshot of a movie with proper resolution and data quality. This lone snapshot showed that filming reactions in biomolecules is feasible at X-ray FELs (Figure 1).

The European XFEL started user operation in the fall of 2017. The facility is designed to produce 27 000 X-ray pulses per second on average, which is more than two hundred times more than at other X-ray FELs. However, the X-ray pulses are not equally distributed, but arrive in bursts that reiterate 10 times per second. Within each burst, the X-ray pulses repeat a million times per second, albeit only for a very short time. Initially, it was unclear how experiments could benefit from this pulse structure. To make the molecular movies, a powerful optical laser that can produce extremely short light flashes was developed and synchronized to the X-ray pulses of the European XFEL. The movie principle works as follows: A reaction is started by a flash from the optical laser and probed after a specific time delay by an X-ray pulse. One can envision this as a synchronized dance between the optical laser and the European XFEL that is filmed by a sophisticated camera. The screenplay was written and executed in spring 2019 by a team of scientists from the USA, Germany, and European XFEL [3].

To cope with the enormous X-ray pulse rates, control experiments were required. As a result, the rate of X-ray pulses that reached the experiment was slowed down to 560 kHz. In addition, it was necessary to determine the time needed for a volume of liquid jet excited by the optical laser to move away in order to avoid exciting the sample twice (about 4 µs, Figure 2a, c-d). In this way, the team succeeded in filming a reaction in a protein at the European XFEL for the first time. The movie consisted of three snapshots, at time delays of 10 ps (Figure 2b), 30 ps, and 80 ps. These snapshots covered the gap between the ultrafast time regime measured at LCLS and slower time scales accessible at synchrotron sources. The pioneering results not only show how to make molecular movies at the European XFEL, but also provide a complete picture of the reaction dynamics in a protein when combined with previous results. They also demonstrate that, ultimately, every single X-ray pulse from the European XFEL may contribute to the data. The research team is looking forward to more movies of reactions in biologically significant proteins and enzymes produced at the European XFEL.

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Figure 1: Reaction in photoactive yellow protein as filmed at LCLS. The figure shows difference electron density maps of the protein's chromophore pocket, the part of the molecule responsible for its colour. Red: Regions from which the electrons move away. Green: Regions to which the electrons migrate.

(a) First difference electron density map with near-atomic resolution at any X-ray FEL, taken 1  $\mu$ s after illumination of the molecule with a nanosecond optical laser pulse [1]. Blue arrows show structural displacements from the initial structure before laser illumination (yellow) to two intermediate states (pR1: magenta, pR2: red).

(b) An ultrafast snapshot taken 3 ps after laser illumination. The chromophore structure changes from a conformation called *trans* (reference structure before illumination, marked in yellow) to one named *cis* (black curved arrow, twisted *cis* structure marked in green) [2].



Figure 2: Data collection for making molecular movies at the European XFEL.

(a) Timing scheme: 564 kHz X-ray pulses from the European XFEL (black) are synchronized to 141 kHz laser pulses (blue).

(b)–(d) Difference electron density maps taken at various delays between laser and X-ray pulse. Red: Regions from which the electrons move away. Green: Regions to which the electrons migrate. (b) Difference electron density map at a delay of 10 ps, (c) 1.78 µs, and (d) 3.56 µs. The map in (b) is very different from (c). In (d), the signal (arrow) is almost gone.

Structures of the chromophore: Before illumination: *trans* (reference structure, yellow); 10 ps after illumination: *cis* (green); µs after illumination: intermediate states (pR1: magenta, pR2: red).

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### STUDYING CAVITATION BUBBLES

Malte Vassholz and Tim Salditt, University of Göttingen, Germany

Small gas bubbles in liquid water can be enjoyed not only in the form of a glass of sparkling water but also in the extreme non-equilibrium states of cavitation bubbles. Such bubbles form when rapid changes of pressure in a liquid lead to the creation of small vapour-filled cavities in places where the pressure is relatively low. The cavities exhibit a range of interesting non-linear effects, from shock wave emission and violent collapse to sonoluminescence, i.e. the emission of light as the imploding shock wave from the collapsing bubble compresses the gas at its centre. Apart from being relevant for fundamental questions, cavitation bubbles are instrumental in a range of important applications, from laser surgery to material processing. In an experiment at the MID instrument of the European XFEL, we used holographic flash imaging with X-ray free-electron laser (FEL) pulses to study cavitation bubbles, seeded by an infrared laser pulse in water, with high spatial and temporal resolution. In contrast to visible light, where strong refraction and multiple scattering make it difficult to probe the interior of the bubble, X-ray imaging offers the unique advantage that it can be used to probe not only the shape but also the interior electron density of the bubble. Knowledge of this density is required to quantify the state of the compressed gas and the shock wave as well as the process of bubble formation from a laser-generated plasma. A fully automated analysis of the radial electron density profile, reconstructed from the measured holograms of about 5000 individual bubbles, gives us access to important physical parameters of the cavitation bubble at various points in time after seeding by the laser pulse.

In this experiment, we studied laser-induced cavitation in water, i.e. the generation of vapour gas bubbles following optical breakdown and plasma formation after focusing a short laser pulse into a water cuvette. The initial supersonic regime of the bubble expansion leads to the emission of a shock wave. The cavitation bubble grows to a maximum radius and subsequently collapses, which may again result in the emission of a shock wave. Over the last decades, several applications of laser-induced cavitation have evolved, ranging from material and surface processing through sonochemistry to medical laser surgery. The formation mechanisms and dynamics of laser-induced cavitation have been studied intensively using optical and acoustical methods [1, 2]. To observe

the cavitation dynamics, imaging techniques with high spatial and temporal resolution are required. Near-field X-ray holography with ultrashort X-ray FEL pulses fulfils these requirements, as it is a single-shot wide-field technique with a spatial resolution up to 20 nm [3].

Figure 1 shows a schematic of the experiment at the MID instrument. An infrared pump laser aligned coaxially with the X-ray beam served to seed cavitation bubbles in a water cuvette placed behind the X-ray focus. The X-ray FEL pulses were used to probe the cavitation bubbles at specific time delays after seeding. Single-pulse holograms were recorded by a detector located behind the X-ray focus. The process was repeated at a rate of 10 Hz, and the time delay was varied to acquire a time series of the cavitation dynamics (Figure 1c).

The X-ray holograms contain guantitative information on the projected phase shift between the X-ray beam that passes the bubble and the empty X-ray beam that serves as reference. This phase shift is directly related to the electron density distribution of the cavitation bubble. To extract this information, wavefront modulations by the empty X-ray FEL beam first need to be separated from the contribution by the bubble. In a second step, the phase shifts have to be recovered by phase retrieval algorithms. The empty-beam correction of holographic recordings with X-ray FEL pulses is considerably more challenging than for synchrotron experiments because the self-amplified spontaneous emission (SASE) process by which the X-ray pulses are generated results in strong pulse-to-pulse variations of the X-ray beam. For this reason, we used an approach based on a principal component analysis to decompose the empty beam in its main eigenmodes, as previously shown for synchrotron radiation [4]. We used two different phase retrieval approaches: an iterative scheme based on alternating projections [5] (Figure 2c) and an algorithm working on the radial intensity distribution for radially symmetric objects (Figure 2b).

Figure 2 shows the results obtained by the workflow described above, as one example out of 5000 evaluated and fully analysed events. The radial density (Figure 2b) of the bubble shows a gradual transition from gas to compressed water in the shock wave. The maximum density in the shock wave is around 1.3 g/cm<sup>3</sup>, corresponding to a pressure of about 1.7 GPa according to



the Tait equation, an equation of state that relates liquid density to pressure. This value and, more generally, the entire density profile can be tracked as a function of the

time delay and the bubble energy.

density distribution  $\rho$  (green, right ordinate). Scale bars: (a, c) 10 µm.

Optical illu

Compound refractive lenses

Microphone

Pump laser

As our experiment shows, the quantitative analysis of near-field diffraction patterns in the holographic regime gives access to the physical conditions of cavitation. The structural dynamics under different conditions (parameters of the liquid, external driving of the cavitation) can be studied in detail using the experimental approach we demonstrated at the European XFEL. Furthermore, the measured density in the shock wave provides an important constraint on the equation of state and for numerical simulations. In a follow-up experiment, we will extend our work to study bubble collapse. To date, we do not know down to which radius the bubble shrinks in the final stages of collapse, which is associated with the strongest compression and with sonoluminescence phenomena.

# Near-field hologram

is placed in the defocus of an X-ray FEL pulse. An infrared laser is focused into the cuvette to seed a cavitation bubble inside the water. The X-ray pulse probes the bubble at a specific time delay after the laser pulse. The X-ray hologram is detected by a

Figure 1: (a) Experimental setup: A water cuvette

(d) Retrieved projected phase shift  $\overline{\varphi}$  from RFP and AP (left ordinate). A two-sphere model is fitted to the RFP result. From this model fit, we obtain the radial mass

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### **OBSERVING MAGNETIC** SWITCHING IN REAL TIME

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Ferromagnetic materials can reverse their local magnetization after exposure to strong, femtosecond laser pulses. Why-and how-this process occurs is one of the big open questions in the field of ultrafast magnetism. In an experiment at the SCS instrument of the European XFEL, we were able to follow the switching dynamics of a ferromagnetic platinumcobalt (Pt/Co) multilayer in real time. We found that a single femtosecond infrared laser pulse can turn a metastable state of uniform out-of-plane magnetization in this material into a dense, disordered array of nanometre-scale, circular domains of locally reversed magnetization. Our time-resolved X-ray scattering experiments reveal that the formation of these socalled skyrmions is mediated by a previously unobserved, transient fluctuation phase on a time scale of 300 ps. The fluctuation phase is reproduced by atomistic simulations, which explain that the rapid topological switching required to reach the skyrmion state is enabled by an effective elimination of the topological switching barrier in the fluctuation phase. This mechanism is not only the fastest way of creating a topological phase but, more generally, the first uncovered mechanism of all-optical switching in a ferromagnetic material.

X-ray free-electron lasers (FELs) enable us to study materials in ways beyond the capabilities of any other technique. This includes access to the intrinsic dynamics and microscopic mechanism of some of the most fundamental physical processes, such as phase transitions. In many cases, rapid phase transitions are intimately linked to the formation of topological defects, as observed, for example, in superfluids [1], ultracold quantum gases [2], charge density wave materials [3], and even the expanding early universe [4]. At the SCS instrument of the European XFEL, we have studied the dynamics of a particularly fascinating phase transition: the transition into a topological phase.

Topological phases are characterized by a ground state of non-trivial global topology. A prototypical topological phase is a magnetic skyrmion phase, which can be

found in thin-film magnetic multilayers with perpendicular magnetic anisotropy. In these materials, a combination of interface-induced chiral spin-orbit interactions and long-range dipolar interactions can stabilize topological skyrmion textures, which appear as circular, black domains in real-space X-ray images (Figure 1a). The topological stability of skyrmions makes them attractive for data storage and data-processing technologies, yet creation and annihilation of skyrmions are required in the data-writing process. Here, we investigate the mechanism and the speed of topological switching. Surprisingly, we find that femtosecond infrared lasers can drive the magnetic system into a fluctuation state in which largescale topological switching progresses on a picosecond time scale, much faster than the previously studied and supposedly much simpler reorientation of magnetic domains [5].

Figure 1 illustrates our experimental approach. Our material is a [Co/Pt]<sub>15</sub> multilayer, which is initially prepared in a field-polarized state. By static imaging at the PETRA III synchrotron light source at DESY and by Lorentz transmission electron microscopy, we confirmed that this material transforms into a skyrmion state upon infrared laser exposure (Figure 1a). At the European XFEL, we followed the dynamics of this topological switching in Fourier space via time-resolved, single-shot, small-angle X-ray scattering. As illustrated in Figure 1b, each data point comprises three X-ray pulses with 60 µs spacing and one infrared laser pulse that was applied before the second X-ray pulse. The newly developed 4.5 MHz DSSC detector allowed us to separately store each scattering pattern. Using these unique capabilities, we could ensure that each data point represented a transition from a uniform spin state (Figures 1a and 1c) to a skyrmion state (Figures 1a and 1e) and record the transient state with unprecedented sensitivity.

Figure 1d shows the transient-state scattering pattern 125 ps after the infrared laser pulse. The scattered intensity is almost uniformly distributed across the detector. Such a scattering pattern corresponds to a random distribution of out-of-plane magnetic moments,



Figure 1: Illustration of the experiment. (a) Topological phase transition from a uniform spin state (left) to a high-density skyrmion state (right). The transition is induced by a single femtosecond infrared laser pulse. The experiment aims to resolve the intermediate state leading to switching. Scale bar: 500 nm. (b) Schematic of the setup. The sample is exposed to the infrared beam on a large area. The Fourier transform of the spin texture is recorded by small-angle X-ray scattering before (c), during (d), and after (e) the laser-induced transition. Scale bar: 0.1 nm<sup>-1</sup>

indicative of a hitherto undisclosed fluctuation phase. The temporal evolution of this fluctuation state, shown in Figure 2a, is governed by two simultaneous dynamics: (i) an increase of the integrated scattered intensity and (ii) a coarsening of the magnetic texture, represented by the concentration of intensity at small scattering angles, that is, low momentum transfer q. Within the first 300 ps, the total scattering intensity reaches 80% of the final-state intensity, indicating that both the reversal of perpendicular magnetic moments and the vertical alignment of these moments across the whole film thickness are completed within this time. Since both effects are key to the nucleation of skyrmions, we conclude that the topological phase is established on a 300 ps time scale. Subsequent coarsening of the texture is mediated by coalescence and condensation of high-energy magnons.

The mechanism of skyrmion nucleation is explained by atomistic simulations, which reproduce the observed scattering signal (Figure 2b), including the existence of the fluctuation phase and the rapid generation of net topological charge in that phase. From these simulations, we understand that the fluctuation phase practically eliminates the topological energy barrier, while the persisting short-range order, in contrast to the paramagnetic phase, enables the formation of a skyrmion seed that must consist of more than one spin. Our results are pivotal to our understanding of topological phases and allow us to generate these phases rapidly and efficiently.

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### WATCHING MOLECULES EXPLODE

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One central aim triggering the development of X-ray free-electron lasers (FELs) has been time-resolved single-molecule imaging. Being able to record a "movie" of chemical reactions with atomic resolution would have a huge impact across a wide range of scientific fields. Accordingly, many different experimental approaches towards reaching this goal have been envisioned, and some have started to be realized within the last decade. In the field of atomic, molecular, and optical physics, two methods have recently seen a big push forward when the SASE3 soft X-ray branch of the European XFEL came into operation. At the SQS instrument, we were able to image an aromatic molecule via Coulomb explosion, depicting its geometrical structure and charge-up dynamics after X-ray ionization. Moreover, making use of electron diffraction imaging, we obtained snapshots of the breakup of oxygen molecules that had absorbed two X-ray photons in the same molecule. Our results suggest that, by carrying out timeresolved experiments in the next step, the dream of recording molecular movies of photochemical processes is close to its realization.

Getting access to the microscopic realm of atoms and molecules has challenged scientists since generations. One rationale behind the development of X-ray FELs was to provide a light source that is capable of illuminating this realm using suitable wavelengths and exposure times [1]. While X-ray diffraction imaging became a key technology for nano-sized samples, other approaches have been pursued for smaller molecules. One intuitive method is Coulomb explosion imaging [2]: The very brilliant X-ray FEL pulses are used to charge up all atoms of a molecule and-due to the Coulomb repulsion of the generated atomic ions-trigger its complete fragmentation. By measuring the emission directions and velocities of all fragments, the molecular geometry can be inferred.

We could demonstrate that, contrary to common belief, recording only a few ions can be sufficient to image a complex molecule and to infer detailed information on the charging and breakup during the femtosecond X-ray pulse [3]. Key to this achievement are the very short and very intense soft X-ray pulses, which allow for an almost instantaneous removal of many electrons. The momentum images obtained with the help of a reaction microscope (see box on p. 19) are of unprecedented quality. Figure 1 shows a momentum map of carbon ions from iodopyridine molecules, allowing the unambiguous identification of every atom of the molecule. The same plot can be created for hydrogen atoms. Those are particularly difficult to observe with other methods because of their low scattering cross sections, but they are crucial players in many photochemical reactions. Being able to investigate protons is thus an important benchmark towards time-resolved studies, e.g. of isomerization reactions.



Figure 1: Ion momentum map of iodopyridine molecules (C5H4IN, see inset). The structure of the molecule is clearly represented in the data, as visualized by the dashed coloured lines. The plot is generated as follows: For all shots in which I2+ (purple), N+ (blue), and at least one C+ (black) ion were created, all ion momenta are normalized such that the magnitude of the I2+ momentum is 1. Then the coordinate system is rotated such that the I2+ momentum points along the z-axis ( $p_x = p_y = 0$ ,  $p_z = 1$ ) and such that the N<sup>+</sup> momentum is in the upper half of the figure ( $p_{v} = 0, p_{v} > 0$ ). The momenta of the N<sup>+</sup> and C<sup>+</sup> ions are then plotted in this coordinate frame.

In addition to ions, other messengers transporting information from the microscopic world are electrons. Like all quantum objects, electrons are not only particles but can also be regarded as waves. Similar to a sonar employing sound waves to sample the surroundings of a submarine, electron waves can be used to image the molecules-thus illuminating the molecule "from within" [4]. The photoelectron wave emitted after the photoionization is scattered by the molecular potential, generating a complex diffraction pattern. By detecting electrons and ions in coincidence, the orientation of the molecule at the time of ionization can be inferred. Figure 2 shows a typical diffraction pattern of an energetic photoelectron emitted from an oxygen molecule. Due to the high photon intensity of the European XFEL X-ray pulses, two photoelectrons can be emitted sequentially from the same molecule. This allowed us to record several electron diffraction images, visualizing the first 20 fs of the molecular breakup; Figure 2 depicts one of these [5].

The results presented here can be considered the first step towards time-resolved imaging of molecular dynamics in the gas phase. We expect these technical advances to open the door to investigating photochemical processes in unprecedented detail. Both methods presented here can, in the future, be used to record "movies" of molecules undergoing structural changes triggered by an external optical laser or a second X-ray FEL pulse.

### **REMI** experiment station at SQS

The reaction microscope (REMI), one of three experiment stations that are part of the SQS instrument, was designed for coincident ion and electron momentum imaging. A REMI employs static electric and magnetic fields to guide ionic particles and electrons towards time- and position-sensitive detectors on opposite sides of a spectrometer (Figure 3) [6]. From the recorded momenta of the particles, their emission directions and energies as well as relative angles can be retrieved. The REMI is a user contribution from the Goethe University Frankfurt in Germany, funded by the BMBF. The team spent two months at the European XFEL working with the SQS group before starting the first experiments, together with a large international group of users.



This highlight article summarizes the results from two of the first user experiments at SQS and was written by the principal investigators on behalf of the respective international collaborations (> 60 persons in total).

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Figure 2: Polarization-averaged photoelectron diffraction pattern from an oxygen molecule. Shown is the second photoelectron emitted in the cascade process, used to probe the molecular potential. The molecule is aligned horizontally, and the electron is emitted from the right oxygen atom. The black dots are the recorded data with statistical error bars, and the blue line is the result of a fit. The diffraction pattern changes strongly as a function of the distance between the two atoms in the oxygen molecule, thus imaging the breakup of the molecule on the femtosecond time scale. The snapshot shown here corresponds to the beginning of the breakup, that is, to internuclear distances of approximately 1.2 Å.

> Figure 3: Sketch of a reaction microscope. The molecules are delivered into the interaction region in a supersonic gas jet. The X-ray pulse from the European XFEL hits one of the molecules, creating multiple ions and electrons. Those are guided towards two time- and position-sensitive detectors on opposite Ihre Post per E-Mail sides of a spectrometer by static electric and magnetic fields. In this way 3D momenta of all recorded particles can be obtained, making it possible to reconstruct the molecular structure by momentum conservation.

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### TAKING SNAPSHOTS OF NANO-STRUCTURES IN SUPERFLUID HELIUM DROPLETS

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Helium droplets are fascinating creations. With a temperature of less than half a degree above absolute zero, they remain liquid, even superfluid—a state in which friction completely vanishes. In this cold environment, embedded dopant particles of atoms or molecules quickly reach their ground state and move freely inside the droplets. When multiple dopants are added, they can coagulate and form very unusual nanostructures. Using the ultrashort, high-intensity X-ray pulses of the European XFEL, we took snapshots of nanostructures formed under these extreme conditions at the new nano-size quantum systems (NQS) experiment station of the SQS instrument.

Equilibrium processes require time to equipartition energy and find the thermodynamically most favourable configuration independent of initial conditions. In an equilibrium state, we can describe why water boils or turns into ice. Our world, however, is made richer by processes occurring far from equilibrium, where structure and pattern formation is controlled by kinetics rather than thermodynamics [1]. The cracking of glass, the formation of snow, and even the assembly of cells in living systems are some of the familiar processes occurring far from equilibrium. However, physical theories describing non-equilibrium systems often only consider factors occurring at the macroscopic level, such as hydrodynamic flows and large-scale turbulence. At the atomic and molecular level, far-from-equilibrium processes are described using macroscopic symmetry scaling laws, which usually neglect the underlying physics on the microscopic scale [1]. This neglect is partly due to the experimental difficulty of studying out-of-equilibrium nanostructures, where particle-by-particle growth is important.

Superfluid helium droplets are unique, self-contained media conducive to growing out-of-equilibrium nanostructures. This viability is due to the droplets' superfluidity, their very cold ambient temperatures of 0.4 K, and the possibility to control the size and composition of embedded dopants, one particle at a time [2]. Superfluid

droplets are produced by expanding pressurized helium into vacuum through a cryogenically cooled nozzle. Dopants are captured by the droplets within the pickup cells along the droplets' flight path. Once a dopant is captured, it quickly thermalizes to the droplet temperature and is decelerated until it moves inside without friction. When several dopants are captured, they coalesce and form far-from-equilibrium nanostructures [2]. While some dopant materials form compact clusters at one or several sites in the droplets, some polar molecules form long linear chains. Other studies have shown a core-shell structure of a multicomponent doped droplet or indicated the formation of foam structures. Up to now, these very special structures could only be inferred from spectroscopic measurements on ensembles restricted to small droplet sizes. Imaging these nano-structures can give us unprecedented insights into the processes underlying their formation.

The technological development of X-ray free-electron lasers (FELs) enables X-ray coherent diffractive imaging (XCDI) of single, non-periodic particles. XCDI has so far been applied to single viruses [3], soot particles [4], large solid xenon clusters [5], and silver clusters [6], among others, with a resolution of a few tens of nanometres. For helium droplets, XCDI was first used by the team of Christoph Bostedt, Oliver Gessner, and Andrey Vilesov to investigate the shapes of rotating helium droplets and the structures of quantum vortices inside the droplets [7]. In vortex-containing droplets, nanostructure formation is dominated by the instant attraction of the dopants to the vortex core. In effect, the dopant structure resembles the shape of the vortex core or vortex lattice. These droplets with quantum vortices were produced from the fragmentation of liquid helium. In order to create and image nanostructures not induced by the vortices, we need to produce large superfluid helium droplets that do not interact with the walls of the nozzle channel, where the initial droplet vorticity is possibly acquired. This may be possible by producing droplets from the condensation of cold helium gas.

The schematic of the experiment setup is shown in Figure 1. The average size of the droplets, which is on the order of hundreds of nanometres, can be controlled by varying the nozzle stagnation pressure and temperature. A skimmer separates the nozzle chamber from the doping region, where different types of doping cells for gaseous, liquid, and solid dopants are installed. In this experiment, xenon, silver, acetonitrile, and iodomethane (the last two of which are polar molecules) are used as dopants. The pure or doped droplets reach the interaction point, where they are intercepted by the European XFEL pulses at a photon energy of 1 keV. Figure 2 shows examples of collected diffraction images of pure and differently doped droplets.

Almost all diffraction patterns from pure droplets exhibit the same concentric ring pattern as the example shown in Figure 2. This observation indicates that the droplets are mostly spherical in shape. In contrast, some of the droplets produced at the liquid fragmentation regime from previous experiments at LCLS in the USA, at FERMI in Italy, and using lab-based high-harmonic generation (HHG) showed extreme shape distortions, e.g. pill shapes or dumbbell shapes [7]. Theoretical work supports the idea that the shape of these distorted droplets is controlled by the presence of quantum vortices: the more deformed a droplet, the larger the possible number of vortices [8]. As the shapes of the droplets produced in our experiment are almost spherical, we can assume that these droplets contain either a small number of vortices or none at all.

A second aspect of our experiment was to investigate structure formation using different types of dopants. The intermolecular interactions (van der Waals, dipole–dipole, or metallic) of these dopants may alter the overall structure growth in the droplet. Our analyses and reconstructions are still ongoing. However, the observed diffraction patterns from different dopant materials in Figure 2 show distinct features. For example, the diffraction patterns collected from droplets with atomic dopants suggest the presence of one to two cluster cores in the droplet. On the other hand, the diffraction patterns from droplets doped with polar molecules suggest a complicated network of dopant clusters.

These imaging experiments at the SQS instrument open novel avenues for further studying different far-fromequilibrium nanostructures in superfluid droplets almost devoid of vortices. Our preliminary analysis also indicates that structure formation can be controlled by the size of the droplets and the properties of the dopants.

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Figure 1: Schematic setup of the helium droplet experiment performed at SQS



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### **NEWS AND EVENTS**

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### 3 JANUARY

### European XFEL to build visitor centre

European XFEL announces it will build a visitor and conference centre with school labs on the Schenefeld campus. Construction is expected to start in 2021. The centre will give the general public the opportunity to learn more about the research at the facility.



Visitors will be able to experience science at the European XFEL visitor centre.

### 23–25 JANUARY Users' Meeting: Leading X-ray researchers meet in Hamburg

With 1100 leading X-ray researchers and nanoscientists from 30 nations, the 2019 joint European XFEL and DESY Photon Science Users' Meeting is held over three days in Hamburg. Participants present new results, investigate possibilities, and discuss the further development of research light sources.



Attendees of the European XFEL Users' Meeting

### 25 FEBRUARY Collaboration starts with local schools

A visit from eighth-grade students of the local school "Achter de Weiden" is the kick-off for further collaboration projects with secondary schools. The goal of the collaboration is to provide pupils from the area with an exclusive look behind the scenes and the chance to engage with staff in order to explore job and apprenticeship opportunities at a scientific institute such as European XFEL.



Eighth-grade pupils visit the European XFEL tunnel.

### **25 FEBRUARY**

### Latvian President Raimonds Vējonis visits European XFEL

Latvian President Raimonds Vējonis visits European XFEL together with more than 30 guests from science, politics, and business. The president participates in a tour of the experiment hall and photon tunnels before taking time to talk to representatives from European XFEL and DESY in a roundtable discussion.



Latvian President Raimonds Vējonis during his visit to European XFEL

### 7 MARCH Sakura Pascarelli appointed scientific director

The Italian physicist Sakura Pascarelli is appointed scientific director at European XFEL. Pascarelli joins the company on 1 September from ESRF in Grenoble, France. She succeeds Andreas Schwarz, who retired at the end of 2018.



Scientific Director Sakura Pascarelli

### 20 MARCH

### Important step towards single-particle imaging

In a model experiment carried out at ESRF, European XFEL scientists, together with international collaborators, come one step closer to successfully carrying out single-particle imaging experiments. The results show that, even with weak signals, an accurate 3D model of the sample can be calculated and that a low level of background noise is vital to achieve good results.



Left: 3D image of a gold sample reconstructed based on the data collected. Right: Reference image of the sample taken with a scanning microscope.

### 28 MARCH

### Girls' and Boys' Day at European XFEL

Twenty-nine girls and boys between the ages of 10 and 14 get a look behind the scenes at European XFEL. The half-day programme includes exciting activities, such as vacuum and crystallization experiments, programming a robot, and build-ing a spectrometer.



Kids build small spectroscopes and learn what scientists and engineers do day to day.

### 24 APRIL Company restaurant opens

The new company restaurant, BeamStop, officially opens. It serves warm meals weekdays from 11:30 to 14:00 as well as snacks and hot and cold drinks until 15:00. It seats a total of 150 guests and is open to European XFEL staff, users, guests, visitors, and the public.



European XFEL Managing Directors Robert Feidenhans'l and Nicole Elleuche serving food in the kitchen of the new company restaurant. Schenefeld's Mayor Christiane Küchenhof (left) is the first to taste one of the prepared meals.

### 29 APRIL Hamburg Prize for Theoretical Physics awarded to Matthias Troyer

The 2019 Hamburg Prize for Theoretical Physics from the Joachim Herz Foundation is presented to Matthias Troyer, a professor at ETH Zürich, Switzerland, and quantum computing researcher at Microsoft. Troyer, who was nominated for the prize by Alexander Lichtenstein, the head of the Theory group at European XFEL, and European XFEL Managing Director Robert Feidenhans'l, plays a key role in the development of quantum computers and superconducting materials. Troyer will use the research stays connected with the prize to collaborate closely with physicists in Hamburg, including at European XFEL.



Quantum researcher Matthias Troyer (middle) during the Award ceremony at Planetarium Hamburg

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### 11 MAY European XFEL at the Science Picnic in Warsaw

More than 50 000 visitors attend the 23rd Warsaw Science Picnic. The event, organized by Radio Poland and the Copernicus Science Centre, takes place around the large PGE Narodowy stadium. The activities at the European XFEL booth of the company's Polish shareholder, NCBJ, are met with great interest. As part of European XFEL's own exhibition, young visitors in particular are keen to virtually explore the FXE instrument, where scientists investigate the sequence of extremely fast reactions and processes.



Warsaw Science Picnic around the PGE Narodowy stadium

### 11 MAY Collaboration agreement with Australian La Trobe University

European XFEL signs a collaboration agreement with La Trobe University in Australia. The six-year programme will focus on joint research projects and co-supervision of Ph.D. students. Research topics will range from understanding the fundamental physics underpinning ultrafast X-ray–matter interactions to probing the real-time dynamics of biological systems at the atomic scale.



European XFEL Managing Director Robert Feidenhans'l (left) and La Trobe University Acting Deputy Vice-Chancellor (Research) Chris Pakes (right)

### 22 MAY

### ATTRACT funds 170 projects to develop solutions for key societal challenges

ATTRACT, a Horizon 2020 research and innovation project funded by the European Union and backed by a consortium of nine partners, including European XFEL, announces 170 breakthrough ideas, each of which will receive 100 000 euro to develop sensing and imaging technologies aimed at changing society. The projects selected for funding were drawn from a pool of more than 1200 proposals from researchers and entrepreneurs in scientific and industrial organizations across the world.



### 28 MAY First experiments with fastest soft X-ray camera in the world

The fastest soft X-ray camera is successfully put through its paces, and the first scientific experiments with the unique DSSC detector have been successfully conducted at the SCS instrument. The installation, commissioning, and operation of the detector mark the culmination of over a decade of international collaborative R&D. The device is designed specifically for the low-energy regimes and long X-ray wavelengths used at the European XFEL soft X-ray instruments and will significantly expand the scientific capabilities of SCS. It will enable ultrafast studies of electronic, spin, and atomic structures at the nanoscale. At full capacity, the DSSC detector can acquire images at a rate of 4.5 million images per second, matching the speed of the X-ray flashes provided by the European XFEL.



European XFEL management and staff celebrate the successful installation and commissioning of the DSSC detector at the SCS instrument.

#### **4 JUNE**

### All six European XFEL instruments are operational

First experiments start at HED, the sixth and final instrument of European XFEL's current design configuration to start user operation. The facility now has the capacity to host three times as many user experiments as it did when operation began in 2017.



First users at the HED instrument

#### 13 JUNE

### Rigid bonds enable new data storage technology

In a paper published in *Science*, a group of scientists led by researchers from European XFEL and the University of Duisburg-Essen in Germany describe how they used the capabilities of the LCLS X-ray laser at SLAC in the USA to show that a transition in the chemical bonding mechanism enables data storage in phase-change materials. The results can be used to optimize such materials for faster and more effective data storage technologies. They also provide new insights into the process of glass formation.

Phase-change materials are used in the latest generation of smartphones, enabling higher storage densities and energy efficiency. Data is recorded by switching between glassy and crystalline material states by applying a heat pulse. Until now, it was not possible to study what happens at the atomic level during this process.



Staff scientist Peter Zalden (left) and colleagues at the FXE instrument at European XFEL

### 20 JUNE DESY and European XFEL strengthen cooperation with Israeli research groups

DESY, European XFEL, and the Israeli National Committee for Synchrotron Radiation intend to cooperate more closely in research with accelerator-based light sources. A one-day workshop of the three institutions on possible collaboration projects takes place on 20 June at the Israel Academy of Sciences and Humanities in Jerusalem, which is also the home of the Israeli Synchrotron Committee.

### 20-23 JUNE X-ray laser comes to town

European XFEL and DESY, together with other Hamburg research institutions, bring "HiTech" to the market square in front of the Hamburg city hall. An exhibition, hands-on activities, and captivating lectures are all part of the four-day science festival "Summer of Knowledge", which involves nearly 40 Hamburg institutions and organizations. The "HiTech Labor" offers visitors insights into the world of research using X-ray light sources. A 1.3 tonne accelerator component is on display, brought especially to the city centre for the event.



### 24 JUNE

### European XFEL plans ultrahigh-speed network connection to Poland

European XFEL and NCBJ in Poland plan to establish the first ultrahigh-speed connection for research data between Germany and Poland. The aim is for the new Supercomputing Centre at NCBJ to be used for the processing and analysis of data generated at the European XFEL. The dedicated network connection will feature a data transfer rate of 100 gigabits per second. With the exception of the higherspeed connection to DESY, this is approximately 100 times faster than the current typical Internet connection between European XFEL and other research institutes.



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### 25 JUNE Royal visit to European XFEL

As part of a two-day stay in northern Germany, Her Royal Highness Princess Maha Chakri Sirindhorn of Thailand visits European XFEL. She is greeted by the managing directors, Robert Feidenhans'l and Nicole Elleuche, before meeting with European XFEL scientists for a discussion of X-ray science and potential collaboration opportunities. During a tour of the facility, she visits the underground experiment hall and one of the photon tunnels.



Her Royal Highness Princess Maha Chakri Sirindhorn of Thailand (centre) talking with European XFEL Administrative Director Nicole Elleuche

### **25 JUNE**

### Third user run successfully completed, fourth starting soon

The third user experiment period at the European XFEL, which ran from November 2018, is successfully completed. The X-ray beam was available for experiments for a total of 18 weeks. Taken together, 28 user experiments were carried out at all six instruments, and 599 users were welcomed to the facility. While only two instruments were operational at the beginning of the run, a further four started operation during the period, so that all six instruments were operational by the end of the run.



### 30 JUNE European XFEL attends ECNS 2019

European XFEL participates in the European Conference on Neutron Scattering in Saint Petersburg, Russia, with a booth. European XFEL scientists explain the research opportunities at the European XFEL instruments. Different virtual reality presentations allow the conference participants to explore the facility and the FXE instrument hutch.



### 5 JULY European XFEL celebrates LGBT STEM day

Friday, 5 July, is the International Day of LGBTQI+ People in Science, Technology, Engineering, and Mathematics (LGBT STEM Day). As an international, science-driven organization, European XFEL values individuality and diversity, and is working hard to ensure a positive and welcoming work environment where everyone, irrespective of religion, cultural background, gender, or sexual orientation, feels safe and is able to be themselves. LGBT STEM Day is celebrated at European XFEL to show support for the LGBT+ community and to indicate that discrimination of any kind is not tolerated.



#### 23 AUGUST

### First high-speed hard X-ray microscopic movies at a free-electron laser

For the first time, at the European XFEL, a group of researchers performs high-speed microscopy using an X-ray laser. The method allows for observations of processes that take place at speeds of up to a few kilometres per second, paving the way for 3D microscopic movies of fast phenomena, with important potential industrial applications. Such movies could show what happens during complex processes with a resolution at the sub-micrometre level, which is less than the diameter of a human hair, while also teasing out hidden internal details.



High-speed hard X-ray microscopy movie showing a glass capillary bursting. Left: Image produced from the experiment. Centre: Direction of motion of the debris, showing the spinning glass fragments and details of turbulence in the water. Right: Velocity of the debris in metres per second.

### 26–30 AUGUST International FEL conference opens in Hamburg

In August, around 400 scientists from around the world attend the 39th international Free-Electron Laser Conference (FEL2019), co-hosted by DESY and European XFEL. The five-day programme at Universität Hamburg highlights recent advances in FEL theory, technologies, and applications.



Hamburg Senator for Science, Research and Equality Katharina Fegebank welcomes the participants to the FEL conference.

### 6 SEPTEMBER Start of apprenticeship training at European XFEL

The first three apprentice trainees start at European XFEL: two future industrial mechanics and one electronics technician. The new trainees will spend a large part of their training in the 400 m<sup>2</sup> mechanics workshop and in the electronics workshop of the warehouse and workshop building.



Oleg Engelmann (trainer), Konstantin Witt (trainee electronics technician), Lorenz Kersting (group leader, Technical Services), Mike Dahlhaus, and Hagen Niemöller (trainees for industrial mechanics)

### 17-21 SEPTEMBER European XFEL at "Highlights der Physik" festival

European XFEL takes part in the annual science festival "Highlights der Physik" in Bonn. Visitors have the chance to learn about the new science facility and experience it first hand with the help of virtual-reality tools. The annual festival, now in its 19th year, is organized in different cities across Germany. This year's theme, "Show Yourself!" ("Zeig Dich!" in German), highlights technologies and research making the invisible visible.



### 2 OCTOBER All SQS experiment stations up and running

The SQS soft X-ray instrument welcomed its first users at the end of 2018. Now, the SQS team and collaborators complete their ambitious plan to install and commission all three experiment stations, each specifically designed for different types of experiments and samples, ranging from atoms and small molecules to large clusters, nanoparticles, and biomolecules.



SQS scientist Rebecca Boll makes final adjustments on the AQS experiment station before the first users arrive at the end of 2018.

### **11 OCTOBER**

Prestigious scientific grant awarded to European XFEL group leader

Together with colleagues from Uppsala University in Sweden and Radboud University in the Netherlands, European XFEL Theory group leader Alexander Lichtenstein is awarded a European Research Council Synergy Grant worth 8 million euro. Over the six-year period of the project, the international team will develop new theoretical foundations to close knowledge gaps revealed by experiments at X-ray FELs.



European XFEL Theory group leader Alexander Lichtenstein

### 9–13 OCTOBER European XFEL in scientific delegation to Armenia

A delegation of scientists from DESY and European XFEL visits research facilities in Yerevan, Armenia. The goal of the trip is to strengthen already existing scientific collaborations and together explore new research opportunities and possibilities. A highlight of the trip is a meeting with Armenian President Armen Sarkissian.



Armenian President Armen Sarkissian greets DESY Director Helmut Dosch and a scientific delegation from European XFEL and DESY.

### 21 OCTOBER Familiar faces at European XFEL

Science journalist Ranga Yogeshwar, German astronaut Ulrich Walter, and peace researcher Götz Neuneck pay European XFEL a visit. The guests learn about the function and applications of the X-ray laser and visit the experiment hall together with Managing Directors Robert Feidenhans'l and Nicole Elleuche.



Science journalist Ranga Yogeshwar together with staff scientist Christina Börne during a tour of the facility

### 6 NOVEMBER European XFEL builds guest house

Diggers move onto the European XFEL campus in Schenefeld to start work on the guest house. The four-storey building will have 58 beds in 55 rooms. It is scheduled to open in 2021.

Since user operation began in September 2017, scientists from across the globe have come to the European XFEL to conduct their experiments over the course of several days. The facility and experiments run in 24-hour operation, so accommodation is important. The guest house will be managed by an experienced hotel manager. The construction costs amount to around 7 million euro.



Administrative Director Nicole Elleuche (left) discusses plans for the guest house with members of the construction team.

### 8 NOVEMBER Shedding light on photosynthesis

In a paper published in *Nature Communications*, an international group of scientists show that the fast X-ray pulse rate produced by the European XFEL can be used to study the structure of membrane proteins, such as those involved in the process of photosynthesis. These results open up eagerly awaited experimental opportunities for scientists studying these types of proteins.

Large proteins and protein complexes are difficult to study with traditional structural biology approaches. They are difficult to crystalize and generally only produce small crystals that are hard to analyse. The extremely fast X-ray pulses generated by the European XFEL now enable scientists to collect large amounts of data from a stream of small crystals in order to develop detailed models of the 3D structure of these proteins.



Basic design of a serial femtosecond crystallography experiment at the European XFEL

#### **18 NOVEMBER**

First molecular movies at the European XFEL

In a paper published in *Nature Methods*, scientists show how to effectively use the high X-ray pulse repetition rate of the European XFEL to produce detailed molecular movies. This type of information can help us to better understand, for example, how a drug molecule reacts with proteins in a human cell or how plant proteins store light energy.



Artistic visualization of a serial crystallography experiment

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### 22 NOVEMBER European XFEL celebrates 10th anniversary

European XFEL celebrates its 10th anniversary. In talks and discussions, participants take stock of a decade of development and achievements at the facility, review the expanding scientific capabilities of the instruments, and share their personal experiences. Around 400 participants attend the event, including European XFEL staff members, guests from politics and business, and representatives from shareholders and partner institutes. In November 2009, representatives of 10 partner countries had signed the European XFEL Convention in Hamburg, entrusting the non-profit European XFEL GmbH with the construction and operation of the facility.



European XFEL Council members, management, and distinguished guests slice the anniversary cake during the event.

### 9 DECEMBER Milestone for extreme-conditions science

The European XFEL opens up new perspectives for high-pressure research: An international team uses the intense laser flashes to heat and analyse samples in diamond anvil cells (DACs) at the European XFEL for the first time. The experiments clearly exceed the scientists' expectations. DACs belong to the standard instruments used by high-pressure researchers. In them, two small and ultrahard diamond anvils compress tiny samples, generating pressures like those prevailing in the interior of the Earth. This way, geoscientists can simulate the conditions inside our planet and obtain important information about its core and mantle.



View into the reaction chamber with a revolver for up to six diamond anvil cells in the centre



### **EUROPEAN XFEL CELEBRATES 10TH ANNIVERSARY**

EUROPEAN

FEL

n 22 November 2019, European XFEL celebrated its 10th anniversary. In talks and discussions, participants took stock of a decade of development and achievements at the facility, reviewed the expanding scientific capabilities of the instruments. and shared their personal experiences. In total, around 400 participants attended the event, including European XFEL staff members, guests from politics and business, and representatives from shareholders and partner institutes.

On 30 November 2009, representatives from 10 partner countries signed the European XFEL Convention in the

Hamburg city hall, entrusting the non-profit European XFEL GmbH with the construction and operation of the international facility. Since then, 12 partner countries have signed the Convention. The first users began to carry out experiments at the facility in 2017. Two years later, all six instruments of the initial design configuration were operational, and the first results had been published.

On the occasion of the 10th anniversary, European XFEL produced a photo book, which can be ordered online. The story 'Giant in the Deep' on the following pages is an excerpt from the book.

"European XFEL stands in particular for the successful international cooperation of numerous European partner countries. Especially in today's times, this is a valuable sign and symbol for the fact that, despite all differences, the European countries are still able to create the conditions for unique high-tech research through joint efforts-for top international research, in which the worldwide scientific and research community will also be able to participate in the future."

Oliver Grundei, State Secretary at the Ministry of Education, Science and Cultural Affairs of Schleswig-Holstein

Our vision that the European XFEL would become a magnet for outstanding researchers has become reality: The largest X-ray laser in the world is making a major contribution to establishing Hamburg as an internationally visible science and innovation metropolis. I would like to thank all those "who have contributed to the success of the European XFEL over the past ten years with their curiosity, determination, and scientific spirit, and wish them all the best for the

Katharina Fegebank, Second Mayor and Senator for Science, Research and Equality of Hamburg

Maria Faury, Chairwoman of the European XFEL Council

many countries have contributed—has taken shape. Now, a

POST CARD

decade after construction started, scientists from all over the world visit the facility for experiments, and we are already Robert Feidenhans'l, European XFEL Managing celebrating astonishing results." Director and Chairman of the Management Board

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Otmar Wiestler, President of the Helmholtz

"Beyond the extraordinary technological performances, what touches me the most is the human adventure, the human capital. I praise those scientists, engineers, technicians, and administrative staff from different countries, industries, and research centres who have been working together to translate a common vision into a reality. I praise the professionalism and true involvement of the management and staff of European XFEL."

"I have watched with pride and excitement how this complex masterpiece to which scientific institutes and companies from

Them Marrow Cale

were thank his my

"On behalf of the entire Helmholtz family, I want to congratulate you on the European XFEL success story. We are very proud that one of our members, DESY, serves as the host lab for your unique research infrastructure. Your first experiments have already demonstrated the fantastic contribution it makes to shaping

Giant in the Deep



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30 November 2009: Representatives of 10 nations sign the convention founding European XFEL.

# **GIANT IN** THE DEEP

he physicists and technicians looked excitedly at the large monitors that lined the long table in front of them. They clicked graphs and curves on the screens, repeatedly changing the settings and studying the effects in the readouts. That's how it had been going on for days. But this evening, it was silent in the gymnasium-sized, neon-lit control room, where 10 men worked at the limits of their concentration.

Then, at 21:19, a tiny orange spot with a sharp border lit up on the blue background of the display. Jubilation broke out. "We jumped up out of our chairs and fell into each other's arms," remembers Jan Grünert, who was in the team. "The joy was immense. It was a really special moment in my life," said the physicist and leader of the X-Ray Photon Diagnostics group. "It was the reward of many years of work put in by hundreds of people."

That was the moment, on 24 May 2017, when a gigantic but highly sensitive machine was brought to life-the most powerful X-ray laser in the world. For the first time, all of the components were working together so that the pulses of hard X-ray light raced through the facility in a controlled manner. From afar, at the start of the facility, a piece of metal was hit with an ultraviolet laser beam

releasing electron bunches. These were compressed and loaded with tremendous energy in an accelerator, before magnets forced them on a slalom course. This generated laser pulses of X-ray light. Ultrastrong and ultrashort. "First lasing"-the machine worked! Operation could begin.

an nations sign the

founding European XFET

"European XFEL" is the name of the research facility of superlatives, an acronym for "X-ray free-electron laser". Almost invisible, it operates underground on the west side of Hamburg. A giant instrument, 3.4 kilometres long, with scientists charging into heretofore uncharted territory in the microcosm. Twelve nations have turned a bold vision into reality: Denmark, France, Germany, Hungary, Italy, Poland, Russia, Slovakia, Spain, Sweden, Switzerland, and the United Kingdom. They finance and operate the giant.

Even so, this is a facility that is open to everyone. The ambitious European project has long been a Mecca for experts from different scientific disciplines, including those from outside Europe. "Scientists from around the world who want to expand the boundaries of knowledge are drawn here," enthuses Robert Feidenhans'l, the Danish managing director and chairman of the European XFEL

Management Board. And so researchers queue up for the chance to push forward their studies here. The X-ray laser makes it possible to view the atomic details of viruses, to follow the formation of molecules, and to probe conditions like those found inside planets.

Although there are free-electron lasers operating with hard X-rays other than the European XFEL-in the USA, Japan, South Korea, and Switzerland-it's the Hamburg machine that generates the most X-ray pulses per second at an extremely high light intensity. Because of this, some experiments can only be performed here. The outstanding properties allow scientists, for example, to film the stages of chemical reactions and the work of biomolecules. These are fascinating glimpses into a world that has so far remained hidden from view.

In northern Germany, the path to being the world's best was long and arduous. The first signs of development of free-electron lasers came from physicists in the 1980s. In the years that followed, those most interested met again and again at international workshops discussing their ideas and sketching concepts for implementation. That gave impetus for realising such a facility somewhere in the world.

Similar conversations were happening at the DESY research centre in Hamburg. At that time, the plan was to construct a 33-kilometre-long superconducting linear accelerator called TESLA so that researchers could trace the elementary building blocks of matter. But financing the project became problematic. "In conversations with the research ministry, it soon became clear that this project had a better chance to become a reality if an X-ray laser was integrated into it," remembered Jochen Schneider, who held the reins for the conception of the laser at DESY from the start. "We planned it with one, and then built a smaller prototype of it"-the world's first free-electron laser in the X-ray range, called FLASH. In 2003, the ministry then decided that TESLA would not receive funding, but a big X-ray laser instead wouldas a European project.

And so the 3.4-kilometre X-ray free-electron laser facility was designed from the DESY campus in a north-westerly direction towards the town of Schenefeld in Schleswig-Holstein. Above all, what dictated these dimensions was the length needed for the accelerator to reach the desired electron energies. In addition, the beam would be split and fanned out five times. And at the end, an enormous



28 August 2017: The Elbphilharmonie, Hamburg's new philharmonic concert hall, greets the new flagship science project, the European XFEL X-ray laser in Schenefeld.

experiment hall would be built with 10 scientific instruments, two per beamline. Its area would be 90 metres by 50 metres—as big as a football field. Above that, offices and laboratories.

First, the funds had to be raised-the costs were estimated at close to one billion euros. What followed were protracted negotiations at the political level. Germany, Hamburg, and Schleswig-Holstein were prepared to take on the lion's share of the costs at 58 percent. The majority of the other interested European states wanted to pay between one and three percent of the costs. Only when the Russians got on board with 27 percent, was everything secure. "It was a very exciting time," says Schneider. "If I woke up at four in the morning, I usually couldn't sleep anymore."

Once all legal hurdles were cleared, representatives of the governments of initially 10 countries signed the "Convention on the Construction and Operation of a European Free-Electron Laser Facility" on 30 November 2009 at the Hamburg city hall. With that, the project was officially rooted in international law. Two other countries joined later.

The construction workers had already started on 8 January 2009. The facility was to comprise an underground branched tunnel system. This was necessary because there was no place above ground, as well as giving local residents additional protection from the radiation once the facility was operational. It would go under streets, houses, commercial areas, a football field, a stable, and a creek. Between 6 and 38 metres deep, depending on the topography above.

Two specially built tunnel boring machines, with respective diameters of 6.17 and 5.58 metres, ate through the ground-but not before the tunnel construction specialists had hung a small case containing a wooden holy figure of Saint Barbara, the patron saint of miners, on the walls of the entrance. Extremely precise work was necessary. For example, the tunnels needed to be built in such a way that they would run continually straight, and not follow the curvature of the Earth like other tunnels do. And to avoid vibrations, the floor of the experiment hall was poured with 2.80 metres worth of concrete. with steel anchors fixed a metre deep into the ground so the groundwater could not push it all back up again. Then came a steel mesh over that, 1.2 metres high. That was filled again with concrete.

After the cement mixers left, the interior outfitters got to work. To be installed was: a 1.7-kilometre-long superconducting linear electron accelerator, to be cooled to -271°C, the longest of its kind in the world. Undulators, which would use magnets to force the energised electrons into a slalom course, thereby generating X-ray radiation. Then apparatuses for monitoring and controlling the electron beam, as well as a system of beamlines that would lead the X-ray beams to the different scientific instruments. Finally the scientific instruments themselves, complete with detectors and data analysers, each instrument optimized for a different area of study. A particular challenge during the installations in the tunnel was to negate the threat posed by tidal forces in the Earth's mantle and faraway earthquakes, both of which cause the facility to move ever so slightly over and over again. The supports for the accelerator and the undulators were constructed specifically to be able to compensate for these movements.

Diverse high-tech for the one-of-a-kind construction came from the partner countries, often as an in-kind contribution rather than financial support. Seventeen institutes in eight countries contributed to the construction of the linear accelerator alone. "Coordinating and holding onto the schedule were at times big problems," says Massimo Altarelli. The Italian physics professor

was the leader of the European XFEL project team and later the first managing director and chairman of the management board. "The technical challenges were extreme, and for the most part, they were overcome," he explains, "but in some cases, some components had to be sent back, and again and again new negotiations and delays." The outfitting of the experiment hall had similar issues. "Due to the large-scale construction boom we had here in Germany at the time, the companies we contracted often subcontracted their work to companies that didn't have enough experience," the physicist said and subtly added: "At times, we really had to put our foot down."

Almost eight years after the beginning of construction, the facility was completed. On 1 September 2017, the official grand opening took place, with high-ranking representatives of the partner countries, Johanna Wanka, the German Federal Minister of Education and Research, and 800 additional guests from around the world. In total, the construction of the X-ray laser had cost 1.25 billion euros. Its operation will cost 117 million euros per year, with currently more than 400 scientists, engineers, and administration staff employed at European XFEL. Another 250 members of staff are employed at the partner institute DESY, who operate the linear accelerator. Everyone involved proudly refers to the performance achieved in the meantime by the megamachine: Every second, the European XFEL will be able to generate 27 000 laser flashes with a brightness that is a billion times higher than that of the best conventional X-ray sources.

User operation began in mid-September 2017. Some 90 experiments were carried out by international research groups by November 2019-first at two and eventually at six scientific instruments. Of the five existing tunnels, two are still empty. More scientific instruments are to follow in the coming years. Working groups are currently discussing what new research possibilities carry the most promise. Meanwhile, Managing Director Robert Feidenhans'l is full of optimism. "We are excited by the scientific and technological progress that the world's most powerful X-ray laser will enable in the coming years," he says.

European XFEL's location will soon become even more attractive. In the neighbourhood of the facility, the City of Hamburg wants to build the "Science City Hamburg-Bahrenfeld", a centre for basic research and applied science, by 2040. Other natural science disciplines at the university will find a home here too. In addition, many flats and recreational areas for students, scientists, and creatives are planned.



The realization of these plans is eagerly awaited here at one of the most modern research facilities in the world. "With the Science City Hamburg-Bahrenfeld, science will fuel the urban development in Hamburg," says Feidenhans'l, "and the Schenefeld campus and its surroundings will also benefit from this energy." The future of research in the Elbe metropolis has only just begun.

Excerpt from the book "European XFEL-Enlightening Science" printed in celebration of the 10th anniversary of European XFEL.

Author: Horst Güntheroth has a Ph.D. in quantum physics and has worked for many years as a science journalist. He has written many articles about the research done at DESY and other particle accelerators.

1 September 2017: Several highranking guests make it official: European XFEL is open for research. Cutting the ribbon are (from left) European XFEL Managing Director Prof. Robert Feidenhans'l; Schleswig-Holstein State Minister of Education, Science, and Culture Karin Prien; Polish Deputy Minister of Science and Education Prof. Łukasz Szumowski; Swiss State Secretary for Education, Research, and Innovation Mauro Dell'Ambrogio; Russian Aide to the President Prof. Andrei Fursenko; German Federal Minister of Education and Research Prof. Johanna Wanka; Hamburg Mayor Olaf Scholz; Swedish State Secretary for Education and Research Karin Röding; British Ambassador to Germany Sir Sebastian Wood; and European XFEL Council Chairman Prof. Martin Meedom Nielsen.

Legot



1 September 2017: Alexander Guda of the Southern Federal University in Russia celebrates his status as one of the first users of the European XFEL with a golden 'entry card' during the inauguration ceremony.

### SHORT HISTORY OF EUROPEAN XFEL

1998: In an international collaboration at DESY, scientists begin to develop and test the technology for the Tera-Electronvolt Energy Superconducting Linear Accelerator (TESLA) project. This technology eventually forms the basis for the European XFEL.

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1980–1984: The idea of a single-pass FEL for short wavelengths is introduced in the works of A M. Kondratenko and F I. Saldin (1980) as well as R. Bonifacio. C. Pellegrini, and L.M. Narducci (1984).

February 2003: The German Federal Ministry of Education and Research (BMBF) announces its plan to realize the X-ray laser facility described in the TESLA TDR supplement. The facility is to be a European project, with Germany meeting about 50% of the costs.

October 2003: The site for the new X-ray laser facility is presented to the public. The facility starts at DESY in Hamburg and reaches to Schenefeld in the neighbouring state of Schleswig-Holstein.

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report (TDR) describing a superconducting linear collider with an integrated X-ray laser facility. ber 2001: The FEL at the TESLA

March 2001: The TESLA collaboration at

DESY publishes the TESLA technical design

Test Facility demonstrates the greatest possible light amplification at 98 nm. A user programme with first experiments starts soon afterwards.

 $(\bullet)$ 



#### 2003

#### 2001 1980 1990 2000 2002 2004

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May 1997: The TESLA collaboration, led by DESY, publishes a conceptual design report for TESLA, a linear collider with an integrated X-ray laser facility.

(•)

XFEL is based.

February 2000: For the first time,

scientists at the DESY TESLA Test Facility

generate shortwave laser light in the ultra-



October 2002: As a supplement to the 2001 TESLA TDR, a TDR is published for an X-ray laser facility with a violet range (80–180 nm) using the pioneering dedicated linear accelerator in a sepa-SASE FEL principle on which the European rate tunnel.

r 2004: Representatives from the states of Hamburg and Schleswig-Holstein sign a treaty that provides the basis for the construction and operation of the X-ray laser facility.

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January 2005: Nine countries—France, Germany, Greece, Italy, Poland, Spain, Sweden, Switzerland, and the UK-sign a Memorandum of Understanding (MoU) for the preparatory phase of the European XFEL facility. By the end of the year, the MoU is also signed by China, Denmark, Hungary, and Russia.

August 2005: User operation begins at the new 260 m long DESY FEL (later renamed FLASH), which is used for studies and technological developments related to future projects, such as the European XFEL.

2006

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July 2006: The DESY XFEL project

team and the European XFEL project

team publish the TDR for the proposed

European XFEL facility, describing the

facility's technical and scientific details.

2005



Meeting is held at DESY, with 260 scientists from 22 countries attending.

launched by the BMBF and representatives from for civil construction follows soon after.

dation of a company to build and run the European XEEL facility

 $(\bullet)$ 2007



June 2007: The European XFEL project is officially 12 partner countries. The launch of the tender process

July 2007: The four-year Pre-XFEL project is launched, with the objective to provide the technical, legal, and financial documents necessary for the foun-



January 2009: Civil construction begins for the European XFEL at sites in Osdorfer Born, DESY-Bahrenfeld, and Schenefeld.

October 2009: The European X-Ray Free-Electron Laser Facility GmbH is officially registered in the Hamburg commercial register.

November 2009: In a ceremony in Hamburg, representatives from 10 countries-Denmark, Germany, Greece, Hungary, Italy, Poland, Russian, Slovakia, Sweden, and Switzerland-sign the European XFEL Convention and Final Act, thus establishing the European XFEL GmbH.

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2009



January 2011: The second tunnel-boring machine starts drilling at the Schenefeld site.

June 2011: The first topping-out ceremony for the European XFEL facility is celebrated on the DESY-Bahrenfeld construction site

June 2011: Based on research at SLAC in the USA and DESY in Zeuthen, scientists demonstrate that the parameters of the X-ray flashes for the European XFEL can be improved beyond the original design.

June 2011: The Pre-XFEL project concludes and all remaining tasks are handed over to the European XFEL GmbH.

July 2011: The boring of the 2010 m long accelerator tunnel for the European XFEL is completed.

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2011

June 2013: The underground civil engineering work for the European XFEL is completed.

September 2013: The installation of the European XFEL injector begins at the DESY-Bahrenfeld site.

December 2013: More than half of European XFEL's 92 undulator segments are fully tuned and awaiting installation in the tunnels.

 $(\bullet)$ 

2013

2008

 $(\bullet)$ February 2008: European XFEL moves into its current headquarters at Albert-

Einstein-Ring 19, near the DESY site.

**December 2008:** Contracts are awarded for the construction of the tunnels and buildings at the European XFEL sites.



### 2010

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July 2010: The first tunnel-boring machine begins to drill the tunnels for the European XFEL. Construction continues on the sites in DESY-Bahrenfeld, Schenefeld, and Osdorfer Born.

November 2010: European XFEL becomes the eighth member of EIROforum.



February 2012: The construction of the 2010 m long accelerator tunnel is completed.

2012

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June 2012: The construction of the tunnel network is completed. Four hundred participants attend an event to celebrate the important milestone.

December 2012: G. Geloni (European XFEL), V. Kocharyan (DESY), E.L. Saldin (DESY), and P. Emma (LBNL) are awarded the Innovation Award of Synchrotron Radiation by the Association of Friends of Helmholtz-Zentrum Berlin (HZB).



May 2014: The first components of the X-ray laser's photon system are installed in the photon tunnels.

2014

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May 2014: Construction of the European XFEL headquarters building (XHQ) in Schenefeld begins.

August 2014: The first completed and tested accelerator module is installed in the tunnel.



January 2017: The first electrons are guided from their initial acceleration point in the facility's injector into the superconducting main linear accelerator, which is cooled to -271°C.

May 2017: European XFEL generates its first X-ray laser light, which has a wavelength of 0.8 nm, at the light source SASE1. At first lasing, the laser has a repetition of one pulse per second.

June 2017: The X-ray beam reaches the experiment hall and the SASE1 instruments SPB/SFX and FXE.

July 2017: European XFEL officially enters the operation phase.

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ber 2017: The European XFEL is inaugurated in an international event with national and international media coverage. User operation starts with two instruments. At the SPB/SFX instrument, the first experiment at the European XFEL begins.



March 2019: The MID instrument starts user operation.

June 2019: The HED instrument starts user operation. All six instruments on all three SASE beamlines are now operational.

July 2019: The DSSC detector, the fastest soft X-ray camera in the world, is installed at the SCS instrument.

August 2019: Scientists demonstrate how to use extremely short X-ray pulses to make the first movies of molecular processes. The experiment is carried out at the SPB/SFX instrument.

**November 2019:** Construction begins for the European XFEL guest house on the Schenefeld campus.

November 2019: European XFEL celebrates its 10th anniversary.

December 2019: At the HED instrument, the first high-pressure experiments exploiting the high repetition rate of the European XFEL are carried out.





February 2018: European XFEL starts operation of the second

X-ray light source, SASE3.

May 2018: European XFEL starts operation of the third X-ray light source, SASE2. For the first time, European XFEL successfully runs all three lights sources in parallel.

July 2018: The European XFEL accelerator reaches its design energy of 17.5 GeV for the first time.

July 2018: First light reaches the SASE3 instruments SQS and SCS.

August 2018: First user results from experiments at the European XFEL are published.

October 2018: First light reaches the SASE2 instruments HED and MID.

December 2018: The SCS and SQS instruments start user operation, doubling European XFEL's experiment capacity.



February 2015: European XFEL holds a topping-out ceremony to celebrate the finished construction of XHQ.

**December 2016:** The injector accelerates the first electrons at the European XFEL, producing a series of bunches that pass through the 45 m long injector beamline in 0.15 ms.

December 2015: By the end of 2015, 59 modules for the main accelerator are installed in the tunnel.

2015



(•)

arch 2016: The installation of all 35 segments of the first of three undulators is completed.

ne 2016: The European XFEL staff moves into XHQ and celebrates with an inauguration event.

July 2016: DESY successfully concludes seven months of tests of the first section of the particle accelerator for the European XFEL. The injector exceeds expectations.

September 2016: The installation of 96 accelerator modules is completed. The 1.7 km long superconducting accelerator is installed in the tunnel and ready to be put into operation.

October 2016: European XFEL begins the commissioning of the 3.4 km long X-ray laser. Representatives of shareholders and govern ments attend a celebration event to mark the occasion.



# FACTSHEET



Factsheet

44



### 239 submitted proposals for 2019 allocation periods





**500** 891 individual users in 2019



193 Ph.D. students among users in 2019

### ELECTRON AND X-RAY BEAMS



Diameter of the electron beam



(comparable to the diameter of a human hair)



10 µS (1/100 000 seconds)

27 000 electron bunches per second





Convention founding European XFEL

Minimum wavelength of the X-ray flashes: **0.06 hillionths** of a metre)

### Smallest focus of the X-ray beam: 11 nm (at the MID scientific instrument)

DATA

11.5 PB raw data generated in 2019 (= 11 500 TB, 11 500 000 GB, 11 500 000 000 MB)

### **BEAMSTOP 2019**



31 879

Sold Franzbrötchen (Hamburg-based sweet pastry)



Sold meals

### ENERGY CONSUMPTION

90.5 GWh (2019) 22 625 households (4 people) = 90 500 People

### PLANTING

Osdorfer Born, Schenefeld, and at the Düpenau creek in 2019

1069 broadleef trees

7444 shrubs









### External guests









### **OPERATIONS**

Operations

In 2019, the last two scientific instruments of the European XFEL successfully started user operation, making all six instruments of the facility fully operational.

After a brief commissioning period, MID and HED welcomed their first users before the summer. Since then, all of the scientific instruments have been scheduling user experiments regularly, following a peer-reviewed selection process for experiment proposals. The simultaneous delivery of X-ray pulses from three FEL light sources (SASE1, SASE2, and SASE3) to three instruments operated in parallel-a worldwide unique trait-became the standard operation mode. Accelerator operation further matured. The facility now regularly provides electron energies from 11 to 17 GeV, generating X-ray pulses with wavelengths down to around 0.6 Å, that is, photon energies up to ~20 keV (at the SASE2 source), and pulse energies up to around 10 mJ (at SASE3). It also achieved extreme flexibility in the bunch pattern, as required for the simultaneous operation of all three FEL sources and the corresponding scientific instruments.

In 2019, the European XFEL accelerator was operated for about 6480 h (Figure 1). More than half of this time was used for X-ray delivery, both for user operation and for internal activities, including instrument commissioning. A guarter of the time was devoted to facility development for the accelerator, the FEL sources, and the photon beam transport systems. Finally, a little less than a fifth of the time was assigned to setup and tuning. This last slot included repair accesses outside the scheduled maintenance periods and the time needed to prepare different accelerator states and delivery modes. Nine weeks were assigned to scheduled shutdowns for maintenance and installation.

The average accelerator availability during X-ray delivery time was above 90%. However, single events caused considerably lower availabilities during four X-ray delivery weeks. The causes differed (power glitches, power failures, cold-compressor failure), but all led to a shutdown of the cryoplant of the accelerator. Restarting the facility after such an event is very complicated and takes at least 24 h. To reduce the vulnerability in this area and cut the number of downtime events. DESY-which is in charge of accelerator operation-started to investigate mitigation scenarios.

The simultaneous operation of the three FEL light sources and delivery of X-ray pulses to three experiments, changing twice a day to serve all six scientific instruments, were started in 2019 and successfully improved over the year (Figures 2 and 3). This worldwide unique mode of operation raised several technical and organizational challenges. The performance of each of the three FEL sources turned out to be interlinked with the tuning of either of the other two. Additional measures were implemented in the accelerator configuration and operation to mitigate these effects. For example, operating the

### **OPERATING HOURS**



Setup, tuning, and unscheduled access Scheduled downtime



Figure 1: Operating hours of the European XFEL accelerator in 2019. The cryogenic system of the accelerator was operated throughout the entire year (8760 h). During this time, 3648 h were dedicated to the delivery of X-ray pulses, 1656 h to facility development, and 1176 h to setup, tuning, and unscheduled access. The remaining 2280 h were scheduled downtime.



accelerator with different radio frequency amplitudes and phases within the one-millisecond-long radio frequency pulse of the accelerating field allowed for independent tuning of the SASE1 and SASE2 sources. The decoupling of SASE1 and SASE3-which are located on the same beamline-could be improved by means of a new kicker magnet in front of SASE3. In general, flexible bunch patterns allowed the X-ray pulse delivery to be tailored to the special needs of the experiments and to make optimal use of the available number of electron bunches.

Operation of the accelerator and X-ray pulse delivery to the instruments at the maximum repetition rate of 4.5 MHz were demonstrated in July 2019, showing the readiness of the accelerator. However, safety concerns and the capability of the instruments to deal with these high pulse rates limited the overall X-ray pulse delivery. While electron bunches amounting to a total electric charge of around 24 C were accelerated in 2019, less than 20% were used for X-ray generation. On the positive side, it was confirmed that the radiation doses observed

in the FEL undulators—the magnetic structures in which the X-ray pulses are generated-are largely caused by spontaneous synchrotron radiation produced by the electrons in upstream undulator segments. This radiation is significantly less harmful than particle losses from the electron bunches.

The operation of the scientific instruments was boosted significantly in 2019. In March, as the fifth instrument to come online, MID started welcoming users. The HED instrument followed in May, so that, from summer 2019, all six scientific instruments were regularly scheduling user experiments. The operation of two instruments at the same FEL source typically involved twelve-hour shifts with beam switching at 8:00 and 20:00, meaning that all the instruments received beam every day. The parallel operation of all six scientific instruments significantly increased the overall acceptance of experiment proposals and the number of users who carried out experiments at the facility (Figure 4). It also meant that the accelerator had to be operated regularly for three FEL sources and that the settings and parameters had to be changed much more frequently.

The six scientific instruments provided a total of 3168 h of the X-ray delivery time to the 56 peer-reviewed user experiment proposals that were allocated beamtime in 2019, including the required setup time. This number included user experiments scheduled in parallel on different instruments. In order to improve performance and commission the various instrument setups and sample environments, all instruments still needed to assign an even larger number of hours of the X-ray delivery time to commissioning and testing. A comparatively small amount of X-ray delivery time was further allocated to in-house research activities, typically focusing on specific developments and meant to boost the overall instrument performance. By decision of the European XFEL management, the FXE, SPB/SFX, and SQS instruments assigned one to two shifts in March to practical training as part of the European large-scale facility course HERCULES.

About 890 users from 255 institutes in 28 countries took part in the user experiments in 2019. The User Office organized two calls for experiment proposals, leading to the allocation of experiments for the first and second half of 2019. In these two calls, 130 / 109 proposals were received, respectively, out of which 35 (27%) / 21 (19%) were finally allocated beamtime for 2019.

### **USER EXPERIMENTS**







### DISTRIBUTION OF USERS





Figure 6: Distribution of users in percentage (%) according to major grand challenges themes (with some of the users participating in more than one experiment)





Figure 7: Distribution of successful proposers according to major scientific areas (with some of the proposers participating in more than one experiment). In 2019, this distribution was much more balanced than it was in 2018, reflecting the fact that all six instruments were operational and thus serving all major scientific applications.



### FACILITY UPDATE

### **CAMPUS DEVELOPMENT**

The development of the Schenefeld campus-the largest of the three sites of the European XFEL-focused in 2019 on improving conditions supporting the operation of the facility. Highlights included the inauguration of the BeamStop company restaurant and cafeteria, the start of construction of the quest house, the operation of the warehouse, and the erection of the undulator hall shell. In addition to the new buildings, myriads of small tasks were completed, supporting daily life on the campus and preparing its further development.

As a user facility, the European XFEL requires an environment that offers its users-who spend most of their time working on experiments-an infrastructure to work, relax, eat, and sleep. A first big step was achieved in April 2019 with the inauguration of BeamStop. This restaurant also includes a cafeteria, which offers breakfast and has a pleasant lounge area for breaks. For the European XFEL staff, BeamStop has become a meeting point to eat together or greet colleagues and guests. The restaurant significantly contributes to the exchange between our staff members and has changed the work culture at European XFEL. In October, we broke ground for the first guest house on our premises. The need to lodge users offsite, sometimes far away from the facility, will be history once we inaugurate this guest house in 2021.

In 2019, we also started operating the warehouse, making the delivery and shipping of goods much easier, and providing storage for material and supplies. The

new undulator hall went from ground-breaking in July to completion of the outer shell by the end of the year. The building will be completed in 2020, and the Undulator Systems group will transfer its magnetic measurement and other development activities from the DESY campus to this building in early 2021. Among other things, this will significantly reduce the daily travel of our staff

Toward the end of 2019, the management board decided to build a new office building in order to move workplaces from temporary office buildings and to relieve pressure on office space in the headquarters building. The new office building will be located to the west of the headquarters and will add office space for 200 persons. Construction is planned to start in 2020, and occupation could start in early 2022. For the planned visitor centre, two competitions were organized, one for the development of the exhibition and one for the building. Detailed planning and tendering will start in 2020. The construction of the hazardous materials and technical gases storage areas will start in 2020 as well. Both will be located near the southeast corner of the headquarters building.

Other activities in 2019 included the completion and improvement of technical infrastructure in the experiment hall and the existing buildings, the further development of campus infrastructure, including a parcel station to enable staff members to receive and send parcels while at work, and intensive planting activities and the completion of the Düpenau creek renaturation project.







Figure 1: Lunch at the BeamStop restaurant



(XHU, under construction), F tunnel entrance buildings (XHE2-4), G guest house (XHU, under construction), H dangerous materials store (XDMS, in development) and technical gas storage (XTGS, in development), I ventilation and air conditioning (XHVAC), J central workshop/stockroom (XHWS), K office building (XHO, in development), L visitor and conference centre, school labs (XHV, in development), M gate house (XHGATE)

### FACILITY DEVELOPMENT

In addition to achieving baseline operation of the accelerator and X-ray systems while conducting the early user programme, we continued facility development by installing additional instrumentation and by enhancing capabilities and boosting performance with new schemes and methods.

### Linear accelerator

In 2019, the accelerator performance could be significantly extended and improved. Routine operation was performed at electron energies of 11.5, 14, and 16.5 GeV with bunch repetition rates of 1, 2.5, and 4.5 MHz. The performance of the delivered free-electron laser (FEL) radiation was significantly improved, in particular at the SASE2 and SASE3 FEL sources. Higher photon and pulse energies were achieved, and effects leading to the systematic change of X-ray pulse properties as a function of the position of the pulse inside the pulse train were identified and reduced.

### Light sources and beamlines

During accelerator shutdowns, new equipment was installed, including self-seeding chicanes at SASE2, a new kicker magnet before SASE3, and tune-up beam stops before all FEL sources. The X-ray beam transport safety systems were upgraded to accept a larger beam power, and the SASE3 undulator section was modified to prepare for the installation of a helical afterburner and an electron beam delay chicane. These developments were performed in close collaboration between DESY and European XFEL.



Figure 1: Hard X-ray self-seeding monochromator at SASE2

A particularly important project was the development, installation, and commissioning of hard X-ray self-seeding monochromators in SASE2. Self-seeding will produce narrower-bandwidth FEL radiation, thereby improving the quality of the FEL beam and increasing its brilliance. At the European XFEL, this will be done by means of two diamond crystal-based monochromators inserted into the SASE2 undulator after Modules 8 and 16 (Figure 1). The double-stage self-seeding will enable operation at higher pulse energies and is expected to provide a cleaner spectral profile. The initial commissioning in 2019 allowed the observation of first narrow-bandwidth FEL radiation at a photon energy of about 8 keV. In 2020, studies will continue, with the aim to provide self-seeded radiation for initial experiments at SASE2 towards the end of the year.

Another FEL source development concerned two-colour operation (operation at two different X-ray wavelengths) and harmonic lasing (lasing at higher harmonics of the fundamental frequency in order to extend the wavelength range of the X-ray radiation). This was first demonstrated at SASE3, and first steps towards two-colour operation at SASE2 were performed.

Another important development was the upgrade of the beam shutters in the tunnels, which are needed to stop the X-ray beam when access to subsequent tunnel sections or experiment hutches is required. All shutters were complemented with diamond-based power absorbers and burn-through monitors. The additional devices will absorb the power of the FEL beams in order to prevent them from reaching and potentially damaging the actual radiation safety beam shutters. Diamond is used for the power absorbers due to its outstanding thermal and mechanical properties. The burn-through monitors ensure that no beam arrives behind the power absorbers. The purpose of the upgrade was to enable operation of the beam transport systems at higher power levels, aiming towards full beam capability, while making sure that the various devices fulfil the specific requirements for

radiation safety devices (Figure 2). In order to completely lift the presently applied beam power restrictions and thereby make the full capabilities of the European XFEL accessible to experiments and users, additional installations will be made in the experiment hutches. This development will begin in 2020.

A third important development regarding the X-ray beam transport was the installation at SASE2 and the commissioning at SASE1 and SASE2 of the high-resolution hard X-ray (HiREX) single-shot spectrometers, in particular their ability to read out FEL spectra with MHz repetition rate (Figure 3). These diagnostic devices measure FEL spectra while the beam is transported to the scientific instruments. They are essential for the performance of the FEL sources, in particular for setting up self-seeding.

#### Scientific instruments

In 2019, user operation started at the MID and HED scientific instruments, located at the SASE2 beamline. Besides serving user experiments, all other instruments were further built up and their performance was improved, in particular SCS and SQS, which started accepting users at the end of 2018.

SQS extended the instrumentation suite significantly by adding two more experiment stations and enabling, towards the end of 2019, pump–probe experiments using femtosecond lasers. The SQS reaction microscope (REMI), developed through a BMBF Verbundforschung grant by the group of Reinhard Dörner at the University of Frankfurt am Main, Germany, and the nano-size quantum systems (NQS) chamber were installed, commissioned, and successfully applied in nine user experiments in 2019. The REMI setup (Figure 4) is dedicated to investigating molecular dissociation dynamics. The analysis of the kinetic energies and momenta of all the emerging particles enables the reconstruction of the molecular geometry and structure, as could be successfully shown in first experiments. The NQS setup allows studies of larger



Figure 2: Upgrade of the beam shutters in the tunnel



Figure 3: HiREX spectrometer with MHz readout capability in the SASE2 beam transport

systems, such as clusters, nanoparticles, and biomolecules. It is equipped with electron and ion spectrometers, combined with an imaging detector for coherent diffraction.

In 2019, a pn-CCD detector was successfully commissioned at SQS, developed by a consortium led by the Detector Operations group at European XFEL. In the future, a DSSC detector will enable the use of MHz repetition rates. In the last experiment at SQS in 2019, applying a new femtosecond 1030 nm laser, a user group made use of the controlled molecule (COMO) sample source, developed by the COMO user consortium headed by Jochen Küpper of CFEL in Hamburg, to study the photo-induced dissociation of pyrrole-water clusters. In combination with the atomic-like quantum systems (AQS) chamber installed in 2018, the initial layout of the SQS instrument was thus completed.

By summer 2019, the Optical Lasers group had finished the installation and commissioning of the SASE3 pumpprobe laser for operation at 1.1 MHz. Synchronized femtosecond optical laser pulses were provided to the SASE3 instruments for in-house commissioning and user operation.



Figure 4: The reaction microscope (REMI) setup at the SQS instrument

At MID, first users arrived in March 2019. During the intense commissioning and testing phase, emphasis had been placed on components and capabilities essential for the first user experiments, such as the nanofocusing setup, the nanosecond optical laser, the crvo-cooled silicon monochromator, and the AGIPD detector (Figure 5, left). In addition, the basic functionalities of the instrument, such as windowless operation by differential pumping, the mechanics of the long detector arm, and the sample environment as well as the control and data acquisition systems had to be verified. For speckle scattering experiments, coherent illumination and detection with sufficient resolution and contrast are needed. Speckle patterns recorded by the AGIPD during instrument commissioning (Figure 5, right) show features caused by self-interference of the coherent beam. They have been used to demonstrate beam coherence, evaluate beam size, and test the detector.

Several of the first experiments required highly specialized sample environments provided by external user groups. At MID, the use of such sample environments is enabled, among other things, by the possibility to remove the sample chamber dome to install user-specific setups. The beamline vacuum is isolated by X-ray-transparent windows, made of diamond or Kapton. This feature was for example used in a pump-probe X-ray holography experiment investigating the dynamics of cavitation bubbles generated by the nanosecond optical laser (see Scientific Highlights, p. 14). The experiments were performed at a photon energy of 18 keV, allowing the X-ray beam to penetrate a glass cuvette and several millimetres of water sample. In 2020, a femtosecond optical laser and an X-ray split-and-delay line will be commissioned, both adding significantly to the portfolio of experimental possibilities at MID.

HED welcomed first users at the end of May 2019 after only a few weeks of commissioning (Figure 6). The first experimental campaigns were used to commission and test the focal properties of the X-ray beam and the operation of the spectrometers in the first interaction chamber (IC1).



tances of 0.2 to 8 m, as indicated by the red arrows. Right: Speckle pattern from porous Vycor silicate glass recorded by the AGIPD detector from a single X-ray pulse.

In addition to the baseline instrumentation, a second interaction chamber (IC2) with a diamond anvil cell (DAC) setup inside was installed and commissioned. IC2 was designed for use with 15-25 keV X-rays in diffraction and time-resolved pulse train measurements. It features a revolver with up to six DACs and is currently equipped with a large-area slow-readout detector, which will be replaced by a 1 Mpx AGIPD detector in the future. The DAC setup enables studies of materials under high pressures of several 10 to 100 GPa and is the first permanently installed setup for high-pressure physics at an FEL. After X-ray commissioning in September 2019, a first user experiment was successfully performed in October 2019.

In summer 2019, the HiBEF user consortium finished the installation of a multi-100 TW laser and completed the beam transport and focusing in IC1. The timing synchronization of the laser pulses relative to the X-ray pulse arrival was measured using the photon arrival monitor in the HED optics hutch to be on the order of 220 fs (RMS). At the end of the year, first full-energy shots with 100 TW intensity on thin-foil targets were performed. These demonstrated that the laser setup, its temporal contrast, and its intensity are within specifications, allowing protons to be accelerated to a kinetic energy of about 17 MeV from the rear side of a 2 µm titanium foil. This laser will become available for first user experiments in 2020. The second large laser system (DiPOLE 100-X) arrived at the end of 2019 from the Central Laser Facility (CLF) in the UK and will be installed and tested in 2020.



Figure 6: Group of the first user experiment at the HED instrument, a community-assisted campaign that showed the capability of HED to perform inelastic X-ray scattering experiments from solids with a spectral resolution of around 45 meV.

### **COMPANY DEVELOPMENT**

The European XFEL has now been operating for two years, including the ramp-up of the scientific instruments and user operation from 2017 to 2019. A review of these initial years of user operation shows that they were a success. Nevertheless, some areas of operation have to undergo detailed scrutiny to further understand where improvements and adaptations are required.

At this point, a number of challenges of full user operation with all six scientific instruments running in parallel have been addressed. The old organizational structure was not commensurate with demand for support and development in a resource-limited environment. Solutions to many of the major operational challenges needed to be found in an organizational structure that focuses on working across group boundaries. During the construction phase, each group had well-defined tasks for building instrumentation. These tasks could, to a large extent, be executed by the groups themselves. With the start of the operation phase, the tasks of all groups shifted towards operating and further developing the instrumentation. This new set of tasks demanded significantly increased collaboration across the groups. Limited human and financial resources made it necessary to prioritize and monitor multiple projects in parallel. Therefore, an internal project was started in 2018 to evaluate and adapt the company structure. Organizationally, the year 2019 was dedicated to addressing this structural transformation and to adapting the corresponding processes.

As a first step, three divisions were established: "Administration", "Experiments and Science", and "Development and Operations". The areas of responsibility of the scientific directors were reorganized and clustered to focus particularly on planning and performing experiments in the Experiments and Science Division, on the one hand, and to properly address operations and machine conditions in the Development and Operations Division, on the other. In the latter, a number of different groups were bundled into two new units-the Data Department and the Instrumentation Departmenteach led by a department head.

In addition, during the scrutiny of the company organization, the European XFEL management identified a lack of coordination between centrally acting groups. This problem was addressed by changing the line manage-

ment in some areas and by creating new groups in a way that enabled them to act horizontally across the company structure to guarantee good communication between groups. Directly reporting to Scientific Director Thomas Tschentscher, two new groups-X-Ray Operations and the Project Management Office-were set up to work in a more horizontal way in order to gain a better understanding of the special requirements within the divisions. They focus on coordination activities and will regularly report to the management board. Also, heads of the two new departments were hired and appointed, respectively; both are currently restructuring their departments to better support user operation.

During 2019, new leadership positions were created, and some existing group leader positions were changed and filled with staff members. These activities resulted in 12 changes within the group leader positions, mainly in the Development and Operations Division, and in the creation of the two new departments mentioned above. Most of these new positions were covered with European XFEL staff members, who successfully used the structural transformation to further develop their own professional careers.

Although the administrative and general support groups were not directly affected by these activities and mainly retained their original composition, groups like Finance, HR, and Legal had to implement structural changes in the administration. In addition, approval procedures were adapted, and staff members were moved to other offices to bring them closer together.

Restructuring is scheduled for completion by the end of 2020. The organization will then be well prepared to meet the challenges of operating the facility for an increasing number of users.



### **BUILDING TRUST**

At the beginning of 2019, the European XFEL Management Board informed staff members about their plans to reorganize the company. One of the biggest visible changes was the establishment of the new Development and Operations Division. One year on, group leaders and directors within the division reflect on a dynamic few months.

For Steve Aplin, 2019 is a year to remember: "That was the year that I established to others, and to myself, that I could be a head of department. I've learned a lot. I've gained a bit of weight and lost a lot of sleep, but I'm proud of what we've achieved!"

Aplin, head of the Data Department, and his colleague Harald Sinn, head of the Instrumentation Department, both took up their new roles during the first half of 2019. Their positions and departments were created as part of the company-wide reorganization initiated at the beginning of the year. Not only did the two have to establish their credibility as managers, they had to shape and define their new roles and responsibilities. With more than 160 employees in the two departments, representing a significant proportion of the company, there were plenty of challenges.

"With these new roles, we both stepped away from hands-on, goal-orientated work into roles that are heavily focused on defining procedures, policies, and strategies," says Sinn. "That was really new for both of us."

"The learning curve was brutal—a bit of a baptism of fire!" says Aplin with a grin. "Every day I am doing something new, something I haven't done before. Handling staff reviews, R&D proposals, timesheets, all on top of understanding the challenges, frustrations, and tasks my staff are dealing with."

But why was there a need for a reorganization of roles, responsibilities, and remit at all? "During the construction phase, groups had their tasks and equipped themselves with people and equipment to get the job done," explains Scientific Director Thomas Tschentscher, who heads the Development and Operations Division, of which Sinn's and Aplin's departments are a part. "Groups were focused and worked well as units. However, as we started user operation and approached full operation, we saw that this was no longer efficient. We were now in the situation where we had to enable the operation of the scientific instruments and other X-ray instrumentation — a new task requiring support and coordinated action by many groups. The investment this required, particularly in terms of human resources, created a conflict with other tasks, such as finishing off instrumentation or software developments. Therefore, we needed to establish new processes. For this, we aimed to bring groups with similar tasks closer together to enhance exchange and enable synergies. The overall goal is to manage operation with less staff, enable more research and development, and make the workload more bearable."

"We could see that people were being overstretched and frustrated," says Managing and Administrative Director Nicole Elleuche, who coordinated the reorganization process. "Processes weren't clear or transparent enough, and people often weren't getting the information they needed when they needed it. It's a challenge in this kind of fast-paced intense work environment to make sure everyone knows what is going on and what the priorities are. Our hope was that the new structure would increase transparency, improve communication, reduce peak workloads, and create a happier, more efficient workforce so that together we can ensure European XFEL is the best science user facility it can be."

### A chance to shape the future

Sinn and Aplin, who represent a completely new level of management, knew what they were getting themselves into and accepted the new challenge with enthusiasm. "This was a chance to shape the future of European XFEL," says Aplin.

Although the two department heads could see the chances a reorganization could bring for the company, not everyone was so keen. "There is a lot of enthusiasm in this company but, at that time, not necessarily for reorganization!" says Sinn. "People were doing fantastic work and working really hard. It wasn't clear how a reorganization could improve people's jobs. It is important that we can show that introducing changes will actually improve things. People have to see the change and effects of those changes."

### First things first

Sinn, who started his new role in March, spent much of the first few months defining procedures and workflows together with management. He also spent time handing over the management of his old group, X-Ray Optics, to **Figure 1:** The first meeting of the extended Management Board with Harald Sinn and Steve Aplin (second and third from left) in May 2019

his successor and, as an interim solution, heading the Undulator Systems group when the previous group leader retired. "This was also a really interesting experience," he says. "I learned a lot about undulators and gained a lot of insights into how the group works as we prepared for the arrival of the new group leader, Sara Casalbuoni. I have a much better feeling for the group now than I might have had otherwise, which is really valuable." Both groups are part of Sinn's Instrumentation Department.

FC.

Aplin, who officially joined the company in June from DESY, was a regular guest on campus from the beginning of the year as he tried to find out what a department head at European XFEL was supposed to do. "I had had a lot of contact with the scientific groups and with groups like the Detector group, where we'd worked on projects together, so I had a good understanding of European XFEL as an outsider. But I needed to develop an insider perspective and that involved talking to people who I had never met before—including Harald!"

Sinn, who has been working at European XFEL for more than 10 years, brought other perspectives and insights to the table that complemented Aplin's experiences. So how important was it to be able to work alongside each other during this period? "Personally, it's been a very positive experience to be able to think about the structures in parallel," says Sinn. "In those first few months, we spent a lot of time sitting together, aligning our views on how things should be done. I think this was a very important phase. We learned a lot from each other."

"When I look back, I imagine it would have been a very lonely place if I had not had a peer to talk to," adds Aplin. "It is so important to have someone to bounce ideas off, to lean on for moral support, or to let off steam with."



### The "middlemen"

Sinn and Aplin are not the only ones who have been defining new workflows and structures since the restructuring process began. The Data Department and the Instrumentation Department are part of the newly created Development and Operations Division, headed by Scientific Director Thomas Tschentscher. In addition to the two departments, newly formed groups focusing on project management and X-ray operations were also established in 2019. Andreas Galler heads the new X-Ray Operations group, which is responsible for ensuring efficient X-ray operation of the European XFEL. "We have a unique situation here, where we have groups of people located physically in guite different places," says Galler. "Those responsible for the European XFEL facility sit at DESY, and the scientists using the instruments are at European XFEL. So there needs to be clear communication between these two groups and a clear understanding of what good operation actually means."

Information was often exchanged bilaterally between individuals. This sometimes led to information gaps and misunderstandings. The X-Ray Operations group will make sure that everyone gets the information needed to make decisions. It will also coordinate the efforts of the accelerator team, the instrument groups, and the groups in the Development and Operation Division in the operation of the facility. "I suppose you could say we will be the 'middlemen'-collecting and assessing information, passing it on for evaluation, and coordinating joint activities." Galler started his new role in June and, much like Sinn and Aplin, spent the first few months defining how workflows and communication flows should work. "Although it's clear what needs to be done, we first have to define the procedures and processes that will allow us to do the job," he says. "Given the complexity of the

facility, it's clear this will be an ongoing process, continually updated and adapted in response to changing operation needs and goals."

The Project Management Office, headed by Gerd Wellenreuther, was also established in 2019. Across European XFEL, there are several projects whose goal is to develop new instrumentation in order to improve the scope and scientific performance of the facility. The Project Management Office will support these projects, for example by providing those working on projects with advice, support, and best-practice tools. "We are really here to help," says Wellenreuther. As a first step, he set about getting an overview of the number of projects from the construction phase still to be completed and what resources they needed. Several new development projects have also been defined and started. The definition of project scope and resource requirements is important for the management to determine a prioritization of new projects in a situation where resources are limited. The Project Management Office will also communicate the status and prioritization of projects. "Achieving more transparency is of key importance to keep people informed and motivated, and I am pleased we can contribute to this," says Wellenreuther.

### "Talk, talk, talk!"

It is, however, one thing to make decisions about changes to group structure and responsibilities, and quite another to ensure that these changes are accepted and implemented by the staff members who are affected. So how do you make sure everyone is pulling together? "Talk, talk, talk!" Sinn and Aplin say in unison. "We talk at least eight hours a day," says Sinn. "I've never done it to that extent before." Within their departments, they set up regular meetings with group leaders as well as with the management board and others to discuss, align views, and ensure everyone has the same information. Another improvement has been the arrival of the new management board secretary, Rena Gebhardt, who takes care of the organizational requirements of the division and, in particular, supports the division director and the department heads. "Since she started, my productivity has gone up!" says Sinn. "She helps us structure our time and even makes sure we eat lunch!" adds Aplin.

### It all comes down to trust

But what is the essential element for successfully changing work processes and the way groups interact? "Basically, it all comes down to trust," says Sinn. "The moment you lose trust, you have to stop working. This is essential for having large groups working together,"

"We're changing things-people's roles and responsibilities," stresses Aplin. "Trust goes hand in hand with understanding. Our group leaders need to trust that we are getting the message across to management effectively. and vice versa. If someone is being critical, you have to trust that this comes with the best of intentions. Maybe you don't agree, maybe you're defending different interests, but we all have the same overarching interestto make the facility the best it can be."

The pair have spent much of the last year working on building up that trust. "It's a continued effort of course to maintain that trust," stresses Sinn. "It needs constant dialogue."

But for all their efforts, plans, discussions, and ideas, have there been any tangible changes in the way people work together? "Oh yes," says Aplin. "I can see it on people's faces. The atmosphere is very different. We're moving from people not wanting to be the problem, or pointing fingers, to people collectively finding solutions. People are feeling more secure and, I think, happier."

### **Collaborative projects**

Sinn and Aplin are also pleased to report about several projects where people from different groups have worked closely and effectively together. "The calibration project, tracked and monitored by the X-Ray Operations group but driven by the Data Department, has been an excellent example of how we can work together," says Aplin.

"The groups within the Instrumentation Department have also been involved in two significant projects this yearthe installation of the seeding monochromator in SASE2 and the upgrade of the shutters," explains Sinn. "I was really happy to see that the group boundaries that used to be so strong have now disappeared. It's a really good sign for the future."





### **BUDGET AND THIRD-PARTY FUNDING**

At the end of 2019, 98% of the European XFEL construction budget was spent. The annual operation budget was 118.6 million euro in 2019 and is going to increase to 132.5 million euro in 2020.

### Budget

Parallel to the operation budget, the investments of the remaining construction budget continued for the SASE2 beamline as well as for the remaining buildings. The management of fixed assets was improved, and the reorganization process was supported by the Controlling group.

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

At the end of 2019, 98% of the total cash budget for construction was spent. The total European XFEL payment budget in 2019 amounted to 144.3 M€. Of this, 118.6 M€ (82.2%) was related to operation and 25.7 M€ (17.8%) was allocated to cover ongoing construction projects. The major part of the remaining construction budget was planned with 18.9 M€ for civil construction and another 3.7 M€ for the completion of the beamlines. In the operation part, the major activity "Beamlines and experiments" had a total budget of 39 M€ (27.0%); certain activities were prioritized to reach their goals in 2019. For "Machine and technical infrastructure", with a total budget of 84 M€ (58%), 58.9 M€ was spent on the operation of the accelerator.

Recurrent costs were the largest part of the costs, with 38% and 55.2 M€, and increased in 2019 due to the reduced construction activities. A similar portion of 53.5 M€ was spent for personnel, including staff from DESY. A quarter was spent for operation and construction. For 2020, an increased annual payment operation budget of 132.5 M€ was approved by the European XFEL Council. Amounts for the finalization of the construction

phase already approved in the previous year will be used and therefore transferred to 2020.

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

### Third-party funding

In 2019, European XFEL participated in 14 research projects, eight of which were funded by Horizon 2020 and Interreg, and five by national funding organizations such as DFG and the German Federal Ministry of Education and Research (BMBF).

The overall income of these projects was 5 M€, of which 80% came from European funding and 20% from national funding. The funds spent by third-party projects amounted to about 1.4 M€ in 2017, 1.4 M€ in 2018, and 0.9 M€ in 2019.

In 2019, 11 staff members were employed exclusively for third-party-funded projects. Three projects ended in 2019, and two new projects were started.

### Total Budget 2019



POST CARD

### Call for R&D projects

In spring 2019, European XFEL issued its first call for photon-based R&D proposals, open only to staff members of European XFEL and DESY.

The call focused on topics relevant to

- Improving and moderately increasing the performance of the baseline installations
- Technically improving user operation
- Further developing the SASE4 and SASE5 beamlines in the future

Thirty-two applications were received, covering a broad range of topics. A total of 14.3 M€ in funding was requested, far more than could be granted. Twelve proposals were awarded funding. Each of the projects will run for a maximum of three years and have an annual budget of up to 300 k€. They will start in 2020 with funding of 2.2 M€ for the first year. The total budget for all the projects within the three years amounts to 4.5 M€.

In order to qualify for funding, projects had to be novel and go beyond routine processes and procedures; they were not restricted to the scientific instruments. Some proposers were invited to re-submit the following year and to show the general feasibility of their project or to include a clarification of the scientific case. The next call for proposals will be issued at the beginning of 2020.

### **QUALITY MANAGEMENT IN SAFETY AND ADMINISTRATION**

Company and individual safety as well as quality management are two crucial topics that are mainly addressed by groups in administration and general support and that are directly connected to the management board. Both are constantly being improved and adapted by the groups to ensure smooth operation.

In 2019, the Safety and Radiation Protection (SRP) group clarified the safety responsibilities for the operation phase between European XFEL and DESY, and the common safety committee (Gemeinsamer Sicherheitsausschuss), which is defined by the Operations Agreement, held its first meeting. Rules of procedure were set up, and the interfaces between the areas of responsibility of European XFEL and DESY were agreed upon. A new electrical safety organization that conforms to the recently issued recommendations for the Helmholtz Association was put in place. Another measure was the formal nomination of group leaders as responsible persons in occupational health and safety. This involved the detailed description of the individual areas of responsibility. Taking the complexity of the European XFEL facility into account, this particular measure serves to clarify and document many of the interfaces and should lead to a safer working environment for employees, users, and contractors,

Quality management at European XFEL has interfaces with many different groups and partners, and the improvements implemented by these groups has led to better results in numerous areas. Only a few of the main achievements, which initiated noticeable changes in processes and task execution, are emphasized here. In 2019, the European XFEL Collaboration Agreement with the Helmholtz Association, which was signed in 2018, began to be implemented. Some of the administrative group leaders were invited to participate in the meetings of "Helmholtz Working Groups".

Within the administration, some groups achieved major improvements or successfully worked on ongoing and important projects. The Procurement group, for example, actively saved 1.35 million euro (M€) through successful tenders and negotiations in 2019, as compared to first estimates and offers. In addition, the Procurement group

successfully executed around 6700 purchases and bigger tenders, such as for cleaning services.

Operation of the warehouse was ramped up during 2019, and the operational concept was finalized and implemented, supported by the newly hired warehouse manager. The warehouse provides additional and well-organized storage space and is now intensively used by European XFEL staff.

In 2019, the asset management system proved its worth when the asset manager conducted the second company-wide recurrent review of asset management activities. IT tools were developed to support the operational requirements of a common platform to collect and maintain the relevant asset knowledge.

In November, the Human Resources group implemented the paperless distribution of salary statements as well as tax and social insurance documents. This means not only a reduction of working time, but also a contribution to sustainability.

Besides of these technical improvements, training was prioritized to meet the increased demand within the company. As a result, training sessions, workshops, mediations, and individual coaching sessions were organized. Together with the works council and the equal opportunity spokespersons, training for "managing diversity" was developed and implemented.

In 2019, European XFEL also started to educate apprentices. In collaboration with the Technical Services group, three young people were hired to perform three-year apprenticeships in mechanical and electronic professions. For 2020, the administration looks forward to the start of the new enterprise resource planning (ERP) system, which will be a milestone in professionalizing our administrative processes and further improving quality management in all areas.

Figures 1 & 2: The warehouse with its



International Collaboration

### INTERNATIONAL COLLABORATION

European XFEL maintains an extensive international research network with partners around the world. In 2019, existing and new collaborations helped to further advance X-ray science and the unique research opportunities at the facility.

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

- ATTRACT project (GA No. 777222): Breakthrough Innovation Programme for a Pan-European Detection and Imaging Ecosystem
- CALIPSOplus (GA No. 730872):
   Convenient Access to Light Sources Open to Innovation, Science and to the World
- EDAX (GA No. 669531): Beating Complexity through Selectivity: Excited state Dynamics from Anti-Stokes and non-linear resonant inelastic X-ray scattering
- EOSCpilot (GA No. 739563): The European Open Science Cloud for Research Pilot Project
- MS SPIDOC project (GA No. 801406): Mass Spectrometry for Single Particle Imaging of Dipole Oriented protein Complexes

CAL IPSOPlus

MS SPIDOC

a LEAPS League of European Accelerator-based Photon Sources

Danosc

• OpenDreamKit (GA No. 676541): Open Digital Research Environment Toolkit for the Advancement of Mathematics

DREAMKIT

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

ATTRACT

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

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

The League of European Accelerator-based Photon Sources (LEAPS) held its second plenary meeting in November, at which more than 120 scientists from the 16 accelerator-based light sources in Europe met to further develop technological and scientific solutions and services



as well as to discuss common strategies with representatives of the European Commission and of national science ministries and research funding agencies.

In June, members of the European XFEL Management Board discussed plans of future collaboration with Russian partners and high-level representatives at the European Conference on Neutron Scattering in Saint Petersburg, Russia.

In August, European XFEL, together with DESY, hosted the 2019 International Free-Electron Laser Conference at the main building of the Universität Hamburg. The Science Senator of Hamburg, Katharina Fegebank, welcomed about 400 experts and students in FEL accelerator science coming from Asia, America, Australia, and Europe.

At the end of January 2019, the Chinese Academy of Science – Helmholtz International Laboratory on Free-Electron Laser Science and Technology proposal was officially started after the signature in Berlin of the act regulating its creation. This joint lab has a budget of 1.2 million euro (M€) per year for five years.

The Socio-Economic Impact of Research Infrastructures report of the Organisation for Economic Co-operation and Development (OECD) using the expertise of European XFEL was published in March 2019. This concluded all past activities of European XFEL for the OECD.

Within the Baltic Science Network initiative, European XFEL experts were asked to provide their insight and suggest measures to improve cooperation in the Baltic Sea region in the field of photon and neutron science. A report was published in February 2019. The follow-up programme, BSN Powerhouse, has received funding. European XFEL is providing scientific support for the mobility programme BARI and will join the organizing committee of the upcoming Baltic States Photon–Neutron Symposium in 2020.

https://www.baltic-science.org/bari/



**Figures 1 & 2:** Initial ion source (left) and aerolens for efficient ion transport (right) of the MS SPIDOC prototype

**Figure 3:** During the 39th International Free-Electron Laser Conference FEL19 at Universität Hamburg



**Figure 4:** More than 150 scientists from the 16 accelerator-based light sources in Europe attended the first LEAPS plenary meeting at DESY.

### **CONTACTS TO INDUSTRY**

In 2019, European XFEL's Industrial Liaison Office (ILO) organized a number of workshops through an international network of clusters and organizations that facilitates contact between big science organizations and industry. Potential suppliers and other interested parties-among them the Association of German Engineers (VDI) – participated in these workshops to show which innovative technologies and services could contribute to the continuous upgrade of the facility. Moreover, workshops were organized for European XFEL scientists and engineers in which experts from industry demonstrated how to write effective specifications. Misunderstandings or poor specifications result in issues and costs on both sides: the scientific facility and the industrial supplier. Improving the communication between them is therefore essential.

In order to explore research opportunities for industry at European XFEL, researchers from different companies were invited to exchange information with our experts and scientists. The guests suggested new ideas for applications, which was extremely interesting for European XFEL's scientific groups. This activity was accomplished both through visits of individual companies and in the framework of conferences that took place in Hamburg, such as BioEurope 2019. In particular, representatives of the company EVOTEC discussed collaboration opportunities with the European XFEL management and scientists. EVOTEC SE is a drug discovery alliance and development partnership company, headquartered in Hamburg, Germany. The proximity of both institutions is advantageous to the exchange of expertise and also an asset for synergic drug development in Hamburg and Schleswig-Holstein. In this context, FELs could be used for the development of enabling technologies that drive radical change in the capabilities of the society. Technical collaboration in a specific case will start in 2020.

An important contact was established with Sosei Heptares, a biopharmaceutical company that develops and produces G protein-coupled receptors (GPCRs) for structure-based drug design and targeted drug delivery. GPCRs are a large protein family of receptors and integral membrane proteins that activate cellular responses to external stimuli through numerous internal signal transduction pathways. Drugs developed for this human superfamily account for almost 40% of all prescription drugs on the market to date and, according to Sosei Heptares,

structure-based drug design has not yet been deployed for these receptors. During a workshop in European XFEL, the potential of X-ray FELs for GPCR research and development was discussed, and a basis for collaboration in the development of a suitable sample environment to collect data on this medically relevant class of material was established. In total, more than 182 people from industry participated in initial meetings to explore possible access to the facility and collaboration possibilities. ILO has informed the staff scientists and engineers about intellectual property protection and subsequent exploitation. The first patent was filed and is awaiting evaluation. These activities are supported by experts in the sector, such as Tutech Innovation GmbH, a private-sector subsidiary of Hamburg University of Technology and the City of Hamburg.

ILO has helped to organize the Big Science Business Forum that will be held in Granada. The event will bring together key suppliers and high-level representatives of various international science institutes, including European XFEL, to explore new possibilities for advancing the development of novel technologies. Moreover, a temporary innovation village will be set up in order to foster technology transfer. A systematic process has been started to evaluate the impact of European XFEL research and development activities on industry by combining data available from different groups, from scientific to administrative ones, for example Finance and Procurement. This monitoring will support the management in the decisionmaking to optimize the innovative impact of European XFEL basic research.



Figure 1: Evotec SE discussed collaboration opportuni-

Figure 2: Tutech GmbH supports European XFEL in intellectual property-related issues.



### **OUTREACH ACTIVITIES**

In 2019, European XFEL reached out to non-expert audiences with events and tours of the facility as well as at a number of public events.

Virtual tours, discussions, and small experiments were popular among visitors to the Warsaw Science Picnic, "Sommer des Wissens" in Hamburg, "Highlights der Physik" in Bonn, and the Christmas Market in Schenefeld. Primary school students visited the facility on "Maus Türöffner-Tag", and secondary school students from the "Faszination Technik Klub" performed experiments in the European XFEL laboratories. As part of a collaboration with the school Gemeinschaftsschule Schenefeld, a group of students visited the European XFEL with a focus on vocational training opportunities.

Over 2400 individual visitors attended one of more than 85 guided tours of the facility. Prominent guests included



Figure 1: Small experiments were popular at the Hamburg "Sommer des Wissens", which had a total of 50 000 visitors.



**Figure 2:** As part of the Hamburg-based programme "Faszination Technik Klub", young technology and science fans were invited to carry out laser diffraction experiments, build their own optical microscopes, and examine leaf and flower samples under an electron microscope.

the President of Latvia, V.E. Raimonds Vējonis, the Princess of Thailand, Maha Chakri Sirindhorn, TV presenter Ranga Yogeshwar, and astronaut Ulrich Walter. The majority of visitors were scientists and university students, with school students and local interest groups also coming to the facility. Due to current limitations on staff and infrastructure, tours mostly focused on university students. In the future, a visitor and conference centre will be able to accommodate a greater number of visitors, including the general public, and allow high school students to spend a full day at the European XFEL and perform their own experiments. The centre will include seminar rooms, two school labs, and an exhibition. The tender processes for architects and exhibition designers began in 2019, and detailed planning will continue in 2020.



Figure 3: A group of students from the local school Gemeinschaftsschule Schenefeld visiting European XFEL in January 2019



Figure 4: The winner participants from the Beamline for Schools competition visited European XFEL on 25 October 2019.

### DIRECTOR'S OUTLOOK

In early 2020, when the first draft of this text was written, the outlook for the year looked bright indeed. With all six scientific instruments operational, we were looking forward to the return of our users after the winter shutdown and to many new experimental breakthroughs and success stories throughout the year.

Since then, however, the SARS-CoV-2 coronavirus pandemic has changed the face of the world-and European XFEL has been no exception.

To protect our staff members and visiting scientists, in March, the spring user run was postponed, the facility was put into safe mode, and the majority of staff began working from home. Our staff members concentrated on activities that did not require their presence at the facility, such as analysing data from previous user experiments, preparing peer-reviewed publications, and further improving the performance of instruments. Collaboration inside and outside the facility was actively maintained to continue the development of new projects at the forefront of science.

Getting the accelerator back to full performance from the safe mode will take at least four to six weeks. We expect the user programme to be shifted by at least half a year, meaning that the activities related in this outlook will extend into 2021.

Before the safe-mode shutdown, all of the scientific instruments at the facility were running well and enabling novel research. However, even after the accelerator is powered back up, there will still be a ways to go before the European XFEL can reach full operation and machine capacity. Many components of the instruments are still being commissioned, and others need yet to be installed. Especially at the last two instruments to start operation, MID and HED, further efforts are required to explore the range of possibilities they can offer. At HED, the HiBEF user consortium has been the driving force behind the installation of two new lasers, which will enable experiments on matter under extreme conditions.

Further technical projects include the installation of pump-probe lasers at all the instruments, which will greatly increase the range of possible experiments.

Over the winter 2019–2020 shutdown, the optics and vacuum groups installed radiation safety monitors and shutters, allowing close to 27 000 pulses per second in the experiment hall for the first time. Data analysis protocols are still not as smooth and powerful as we would like and need to be improved. We will also work on reducing the amount of data stored for a more sustainable approach to handling the huge amounts of data the experiments produce.

One of our goals is to increase the amount of time we can make available for user experiments. As we learn more about the instruments, experiments and beamtime can be run more efficiently. With time, we will better understand the range and diversity of the types of experimental setups required by users, allowing instrument groups to standardize and streamline experiment protocols. Types of experiments can be scheduled together to minimize setup times and free up time for the actual experiments. To a certain extent, these steps are already being taken, but clearly there is still work to be done.

User experiences and expertise are crucial for shaping the facility, and we are keen to work more closely with our user communities. We want to improve the dialogue with users to learn even more about their research interests and requirements, discuss their feedback, and take advantage of their expertise. We also want to open channels that enable us to communicate more clearly what they can expect from the facility as they prepare their proposals and to ensure that they get the help and feedback they need. Establishing contact with the instrument groups before writing and submitting proposals means that constructive discussions about the design and scope of the experiments can be worked into the proposals, increasing positive outcomes. We hope this will also encourage more groups new to X-ray FEL science to apply for beamtime. We plan to improve contact with our user communities via a variety of channels, such as the newly established European XFEL



Robert Feidenhans'l, Managing Director and Chairman of the Management Board

User Organization as well as online town hall meetings, where we will directly address users in different regions.

User experience also goes beyond the walls of the instrument hutches. The opening of our company restaurant "BeamStop" in 2019 was a welcome addition to our campus for users, staff, and visitors, giving all of us a place to meet, relax, and recharge after long working hours. Currently under construction, our guest house will have 58 beds in 55 rooms. We will also see the opening of the almost-completed undulator hall, which will be set up for the testing and calibration of undulator modules.

As our current suite of instruments becomes more established, it is time to think about further expanding the scope of the facility. The planned SASE4 and SASE5 beamlines represent new opportunities for additional types of experiments; here again, input from the user community is vital. There are many ideas about the science these beamlines could enable, and we look forward to discussing them in workshops with our users across the shareholder countries.

Looking at the European XFEL in a global and political context, the facility has the potential to make a real impact on the grand challenges facing our society in terms of health, technology, and climate. We are keen to utilize this potential, in close cooperation with our users around the world, to contribute to the positive well-being and development of our society and environment, especially in light of the health challenges the world is facing today.



### AT A GLANCE

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

**Brilliant X-ray flashes for new research opportunities** With a repetition rate of up to 27 000 pulses per second and an outstanding peak brilliance, the world's largest X-ray laser produces ultrashort X-ray flashes that allow researchers to map the atomic details of viruses, decipher the molecular composition of cells, take three-dimensional images of the nanoworld, film chemical reactions, and study processes like those occurring deep inside planets. The European XFEL is located mainly in tunnels 6 to 38 m underground. The 3.4 km long facility runs from the DESY research centre in Hamburg to the town of Schenefeld in the German federal state of Schleswig-Holstein (Figure 1). The facility comprises three sites: the DESY-Bahrenfeld site with the injector complex, the Osdorfer Born site with one distribution shaft, and the Schenefeld campus site, which hosts the underground experiment hall with a large laboratory and office building on top. The latter serves as the company headquarters. Germany (federal government, city-state of Hamburg, and state of Schleswig-Holstein) covers 58% of the costs. Russia contributes 27%, and each of the other international shareholders between 1% and 3%. To a great extent, the European XFEL facility was realized by means of in-kind contributions by shareholders and partners.

As of December 2019, 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 costs for the facility in 2019 amounted to 118.4 million euro. The construction costs, including commissioning, amounted to 1.25 billion euro (at 2005 price levels).

#### Stat

### **STAFF**

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

### STAFF STATISTICS

In 2019, the European XFEL workforce grew from 443 (December 2018) to 470 (+6.09%).

The number of employees grew as follows:

**GENDER SPLIT-UP** 

ALL AND ALL ALL	11
219	(+13
120	(+6
59	(+0
72	(+8
	219 120 59 72







### STAFF DEVELOPMENT



																			6		6	6			
-	lan 18	eb 18	Aar 18	Apr 18	lay 18	Iun 18	Jul 1	vug 18	spt 18	Dct 18	lov 18	Dec 18	lan 19	eb 19	Aar 19	Apr 1	lay 1	Iun 1	Jul 1	vug 19	ept 1	Dct 1	lov 1	Dec 1	

### **TOTAL STAFF**

50 CITIZENSHIPS IN TOTAL (INCL. 12 DOUBLE CITIZENSHIPS)



### SCIENTIFIC STAFF

36 CITIZENSHIPS IN TOTAL (INCL. 8 DOUBLE CITIZENSHIPS)







### Germany Italy Russia Poland, United Kingdom China France India, Iran, Korea, Slovakia, Sweden, Ukraine, USA Brazil, Spain Australia, Denmark, Hungary, Switzerland

Algeria, Canada, Chile, Congo, Czech Rebublic, Egypt, Georgia, Greece, Jordan, New Zealand, Portugal, Romania, South Korea, Uzbekistan, Yemen Shareholders

### **SHAREHOLDERS**

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

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

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

### MANAGEMENT, COUNCIL, **AND COMMITTEES**

### European XFEL Council

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

Chairperson

Maria Faury (CEA, Paris)

Delegates	Denmark	Morten Scharff (Danish Agency for S						
		Copenhagen)						
	France	Pascal Debu (CEA, Paris)						
		Emmanuelle Lacaze (CNRS, Paris)						
	Germany	Volkmar Dietz (BMBF, Bonn)						
		Helmut Dosch (DESY, Hamburg) Györgyi Juhász since 15 September						
	Hungary							
	A set	Development and Innovation Office, I						
	State State State	Dénes Lajos Nagy until 14 Septemb						
		Physics, Budapest)						
		György Vankó since 15 September 2						
		Physics, Budapest)						
	Italy	Carlo Pagani (INFN, Milan)						
		Corrado Spinella (CNR, Rome)						
	Poland	Mateusz Gaczyński (Ministry of Scie						
		Grzegorz Wrochna (NCBJ, Otwock-						
	Russia	Mikhail Kovalchuk (NRC KI, Moscov						
		Andrey Anikeev (Ministry of Education						
	Slovakia	Karel Saksl (Institute of Materials Re						
		Pavol Sovák (P.J. Šafárik University,						
	Sweden	Lars Börjesson (Chalmers University						
		Johan Holmberg (Swedish Research						
	Switzerland	Laurent Salzarulo (State Secretariat						
		Innovation, Bern)						
		Gabriel Aeppli (PSI, Villigen)						
	United Kingdom	James Naismith (Rosalind Franklin I						
		Neil Pratt (UKRI, Swindon)						
Observers	Spain	Miguel Ángel García Aranda until 28						
		Guadalupe C. de Córdoba Lasunci						
		Universidades, Madrid)						
Secretary	Malte Laub (Europ	ean XFEL, Schenefeld, Germany)						
Vice Secretary	Meike Flammer (E	uropean XFEL, Schenefeld, Germany)						

Vice Chairperson

**Martin Meedom Nielsen** (DTU, Kongens Lyngby)

h Agency for Science and Higher Education,

is) CNRS, Paris) Bonn) Hamburg) 15 September 2019 (National Research, vation Office, Budapest) til 14 September 2019 (Wigner Research Centre for

5 September 2019 (Wigner Research Centre for

Ministry of Science and Higher Education, Warsaw) ICBJ, Otwock-Świerk)

RC KI, Moscow)

stry of Education and Science, Moscow)

f Materials Research, SAS, Košice)

rik University, Košice)

ners University of Technology, Gothenburg)

edish Research Council, Stockholm)

ate Secretariat for Education, Research and

lligen) alind Franklin Institute, Didcot) don)

Aranda until 28 October 2019 (University of Malaga) doba Lasunción (Ministerio de Ciencia, Innovación y

**Nicole Elleuche** 

### Management Board

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

Managing Director Robert Feidenhans'l and Chairperson

Managing and Administrative Director

Scientific Directors Serguei Molodtsov and Proxy Holders

**Thomas Tschentscher** Sakura Pascarelli (since 1 September 2019)

Administrative and Finance Committee (AFC)

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

Chairperson	Xavier Reymond (Stat
	for Education, Researc
	tion Down Outbouldered

te Secretariat ch and Innovation. Bern. Switzerland)

Vice Chairperson Neil Pratt (UKRI, Swindon, United Kingdom)

Delegates	Denmark	Morten Scharff (Danish Agency for Science and Higher Education,					
	•	Copenhagen)					
	France	Sébastien Borel until 15 September 2019 (CNRS, Paris)					
		Stéphanie le Van since 16 September 2019 (CNRS, Paris)					
		Salah DIB (CEA, Paris)					
	Germany	Andreas Volz (BMBF, Bonn)					
		Christian Harringa (DESY, Hamburg)					
	Hungary	Györgyi Kolossváryné Juhász (NKFIH, Budapest)					
	Italy	Veronica Buccheri (INFN, Milan)					
		Antonella Tajani (CNR, Rome)					
	Poland	Zbigniew Golebiewski until 2 June 2019 (NCBJ, Otwock-Świerk)					
		Michał Wójtowicz until 3 June 2019 (NCBJ, Otwock-Świerk)					
		Michał Rybiński (Department of Innovation and Development at the					
		Ministry of Science and Higher Education, Warsaw)					
	Russia	Valeriy Nosik (NRC KI, Moscow)					
	Slovakia	Pavol Sovák (P.J. Šafárik University, Košice)					
	Sweden	Hanifeh Khayyeri (Swedish Research Council, Stockholm)					
	Switzerland	Peter Allenspach (PSI, Villigen)					
		Doris Wohlfender-Bühler (State Secretariat for Education, Research					
		and Innovation, Bern)					
	United Kingdom	Neil Pratt (UKRI, Swindon)					

Machine Advisory Committee (MAC)

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

Chairperson

Andrzej Wolski (University of Liverpool, United Kingdom)

Members

Camille Ginsburg (Fermilab, Batavia, Illinois, USA) Ángeles Faus-Golfe (University of Valencia, Spain) Evgeny Levichev (BINP, Novosibirsk, Russia) Heung-Sik Kang (Pohang Accelerator Laboratory, South Korea) Franz-Josef Decker (SLAC, Menlo Park, California, USA) Luca Giannessi (Elettra Sincrotrone Trieste, Italy) Caterina Biscari (ALBA Synchrotron Light Source, Barcelona, Spain) Peter Michel (HZDR, Dresden, Germany) Thomas Schilcher since 24 October 2019 (PSI, Villigen, Switzerland)

### Scientific Advisory Committee (SAC)

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 and its full and effective utilization as well as on future developments required to maintain the scientific and technical productivity of the facility at the highest possible level.

Chairperson

Ian Robinson (University College London, United Kingdom)

Members

Olga A. Olekseeva (IC RAS, Moscow, Russia) Mike Dunne (SLAC, Menlo Park, California, USA) Stefan Eisebitt (MBI, Berlin, Germany) Guillaume Fiquet (IMPMC, Paris, France) Gerhard Grübel (DESY, Hamburg, Germany) Maya Kiskinova (Elettra Sincrotrone Trieste, Italy) Inari Kursula (University of Bergen, Norway; University of Oulu, Finland) Anders Nilsson (Stockholm University, Sweden) Henrik Lemke (PSI, Villigen, Switzerland) Keith Nugent (The Australian National University, Australia) Alexander Popov (ESRF, Grenoble, France) Christoph Quitmann (RI Research Instruments GmbH, Bergisch Gladbach, Germany) Ilme Schlichting (MPI for Medical Research, Heidelberg, Germany) Linda Young (ANL, Argonne, Illinois, USA)

Secretary

Gianluca Geloni (European XFEL, Schenefeld, Germany)

Secretary

Detector Advisory Committee (DAC)

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

Chairperson Jörn Wilms (University of Erlangen, Germany)

Members Branden Allen (Harvard College Observatory, Cambridge, USA First term starting with 26th DAC, 24-26 April 2019 Gabriella Carini (Brookhaven National Laboratory, Upton, USA) First term starting with 26th DAC, 24-26 April 2019 Paula Collins (CERN, Geneva, Switzerland) First term starting with 26th DAC, 24-26 April 2019 Rob Halsall (STFC, Swindon, United Kingdom) First term starting with 26th DAC, 24-26 April 2019 Mark Heron (Diamond Light Source, Oxford, United Kingdom) First term starting with 26th DAC, 24-26 April 2019 Roland Horisberger (PSI (retired), Villigen, Switzerland) Christopher J. Kenney (SLAC, Menlo Park, California, USA) Last meeting: 27th DAC, 9-11 December 2019 Michael Krumrey (Physikalisch-Technische Bundesanstalt, Berlin, Germany) First term starting with 26th DAC, 24-26 April 2019 Kay Rehlich (DESY (retired), Hamburg, Germany) Darren Spruce (MAX IV. Lund, Sweden) First term starting with 26th DAC, 24-26 April 2019

### Laser Advisory Committee (LAC)

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

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

Chairperson

Jonathan Zuegel (University of Rochester, USA)

Members Miltcho Danilov (Elettra Sincrotrone Trieste, Italy) Thomas Dekorsy (German Aerospace Centre, Stuttgart, Germany) Alan Fry (SLAC, Menlo Park, California, USA) Patrick Georges (Institut d'Optique, Paris, France) Catherine Le Blanc (Laboratoire LULI, Ecole Polytechnique, France) Emma Springate (STFC Rutherford Appleton Laboratory, United Kingdom) William E. White (SLAC, Menlo Park, California, USA)

Secretaries Nele Müller (DESY Photon Science, Hamburg, Germany) Andreas Galler (European XFEL, Schenefeld, Germany)

### Proposal Review Panels

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

### FXE Proposal Review Panel

Chairperson

Villy Sundström (Lund University, Sweden)

Members

Michael Wulff (ESRF, Grenoble, France) Shin-ichi Adachi (High Energy Accelerator Research Organization, KEK, Japan) Frank de Groot (Utrecht University, The Netherlands) Thomas Elsässer (Max Born Institute, Berlin, Germany) Jerome Hastings (SLAC, Menlo Park, California, USA) Adela Muñoz Páez (University of Sevilla, Spain) Sylvain Ravy (Laboratoire de Physique des Solides, Orsay, France) Alexander Soldatov (Southern Federal University, Rostov-on-Don, Russia) Metin Tolan until February 2019 (Technical University Dortmund, Germany) Majed Chergui until February 2019 (Ecole Polytechnique Federale de Lausanne, Switzerland)

### HED Proposal Review Panel

Chairperson

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

### Members

Michael Armstrong (LLNL, Livermore, California, USA) Alessandra Benuzzi-Mounaix since September 2019 (Laboratoire pour l'Utilisation des Lasers Intenses, LULI, Paris, France) Guillaume Figuet (IMPMC, Paris, France) Zahirul Islam (Argonne National Laboratory, Lemont, Illinois, USA) Matthias Marklund (Chalmers University, Umea, Sweden) David Neely (Central Laser Facility, Didcot, United Kingdom) Paul Neumayer (GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany) Norimasa Ozaki (Osaka University, Japan) Sergey Pikuz (Joint Institute for High Temperatures, Moscow, Russia) Sakura Pascarelli Chairperson until February 2019 (ESRF, Grenoble, France)

### Vice-Chair

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

MID Proposal	Review Panel	SPB/SFX Prop	oosal Review Panel
Chairperson	Giulio Monaco (University of Trento, Italy)	Chairperson	Inari Kursula (University of Bergen, Norway,
Members SCS Proposal I	David Le Bolloc'h (Laboratoire de Physique des Solides, Orsay, France) Paul Fuoss (LCLS, SLAC, Menlo Park, California, USA) Henrik Lemke (PSI, Villigen, Switzerland) Bridget Murphy (Christian-Albrechts-University zu Kiel, Germany) Anton Plech (KIT, Karlsruhe, Germany) Ian Robinson (UCL, United Kingdom) Anatoly Snigirev (Immanuel Kant Baltic Federal University, Kaliningrad, Russia) Michael Sprung (DESY, Hamburg, Germany)	Members	Gyula Faigel (Wigner Research Centre of Phy Budapest, Hungary) Sébastien Boutet from September 2019 (LC Elspeth Garman (University of Oxford, Unite Cameron Kewish (Australian Synchrotron, C Victor Lamzin (EMBL, Hamburg, Germany) Thomas Möller (Technical University Berlin, C Christian Riekel (ESRF, Grenoble, France) Jozef Uličný (Safarik University Košice, Slova Manfred Weiss from September 2019 (Helm Energie HZB, Germany) Sine Larsen Chairperson until February 2019 Christian Schroer until February 2019 (DES)
Chairperson	Jan-Erik Rubensson (Uppsala University, Sweden)	SQS Proposal	Review Panel
Members	Claudio Masciovecchio (Elettra Sincrotrone Trieste, Italy) Nicholas Brookes (ESRF, Grenoble, France) Manuel Guizar-Sicairos (PSI, Villigen, Switzerland) Simo J. Huotari (University of Helsinki, Finland) Philip Hofmann (University of Aarhus, Denmark) Steven Johnson (ETH Zürich, Switzerland) Alexey Kimel (Radboud University, Nijmegen, the Netherlands) Maya Kiskinova (Elettra Sincrotrone Trieste, Italy) Jan Lüning (University Pierre et Marie Curie, Paris, France) Marcin Sikora (AGH University of Science and Technology, Kraków, Poland) Ian McNulty until February 2019 (MAX IV, Lund, Sweden)	Chairperson Members	Eckhardt Rühl (Freie Universität Berlin, Gern John Costello (Dublin City University, United John D. Bozek (Synchrotron SOLEIL, Gif-su Carlo Callegari (Elettra Sincrotrone Trieste, It Alexei Grum-Grzhimailo (Lomonosov Moso Jon Marangos (Imperial College, London, Un Thomas Pfeifer (MPI for Nuclear Physics, He Stacey L. Sorensen (Lund University, Swede Frank Steinkemeier (University of Freiburg,

and University of Oulu, Finland)

hysics, Hungarian Academy of Sciences,

CLS, SLAC, USA) ed Kingdom) Clayton, Australia) Germany) vak Republic) from September 2019 nholtz-Zentrum Berlin fur Materialien und

9 (University of Copenhagen, Denmark) Y, Hamburg, Germany)

many)

d Kingdom) Ir-Yvette, France) Italy) cow State University, Russia) Inited Kingdom) eidelberg, Germany) en) Germany) Linda Young (Argonne National Laboratory, Lemont, Illinois, USA) Beata Ziaja-Motyka (CFEL, Hamburg, Germany)



### PUBLICATIONS

### **User** Publications

Evaluation of serial crystallographic structure determination within megahertz pulse trains O. Yefanov et al. Struct. Dyn. 6, 064702 (2019) doi:10.1063/1.5124387

Initial observations of the femtosecond timing jitter at the European XFEL H.J. Kirkwood et al. Opt. Lett. **44** (7), 1650–1653 (2019) doi:10.1364/OL.44.001650

Membrane protein megahertz crystallography at the European XFEL C. Gisriel et al. Nat. Commun. **10** (1), 5021 (2019) doi:10.1038/s41467-019-12955-3

MHz data collection of a microcrystalline mixture of different jack bean proteins M.L. Grünbein et al. Sci. Data 6 (1), 18 (2019)

Time-resolved serial femtosecond crystallography at the European XFEL S. Pandey et al. Nat. Methods **2019**, (2019) doi:10.1038/s41592-019-0628-z

### Staff Publications

A post-translational modification of human Norovirus capsid protein attenuates glycan binding A. Mallagaray et al. Nat. Commun. **10** (1), 1320 (2019) doi:10.1038/s41467-019-09251-5

**A superradiant THz undulator source for XFELs** T. Tanikawa et al. J. Instrum. **14** (05), P05024 (2019) doi:10.1088/1748-0221/14/05/P05024

A versatile liquid-jet setup for the European XFEL J. Schulz et al. J. Synchrotron Radiat. **26** (2), 339–345 (2019)

doi:10.1107/S1600577519000894

Ab initio simulations of complementary K-edges and solvatization effects for detection of proton transfer in aqueous 2-thiopyridone J. Norell et al. J. Chem. Phys. **151** (11), 114117 (2019) doi:10.1063/1.5109840

Accelerator beam dynamics at the European X-ray Free Electron Laser I. Zagorodnov et al. Phys. Rev. Accel. Beams 22 (2), 024401 (2019) doi:10.1103/PhysRevAccelBeams.22.024401

### Alignment of the aberration-free XUV Raman spectrometer at FLASH M. Biednov et al.

J. Synchrotron Radiat. **26** (1), 18–27 (2019) doi:10.1107/S160057751801576X

An In-situ Transmission X-ray Microscope to Observe the Dewetting Process of Au Thin Films induced by Nanosecond Pulsed Laser Irradiation S.Y. Lee et al. J. Korean Phys. Soc. **75** (7), 523–527 (2019) doi:10.3938/jkps.75.523

Angular X-ray Cross-Correlation Analysis (AXCCA): Basic Concepts and Recent Applications to Soft Matter and Nanomaterials I. Zaluzhnyy et al. Materials 12 (21), 3464 (2019) doi:10.3390/ma12213464

Atomically thin oxide layer on the elemental superconductor Ta(001) surface R. Mozara et al, Phys. Rev. Mater. **3** (9), 094801 (2019) doi:10.1103/PhysRevMaterials.3.094801

Characterization of the ePix100a and the FastCCd semiconductor detectors for the European XFEL I. Klačková et al. J. Instrum. 14 (01), C01008 (2019) doi:10.1088/1748-0221/14/01/C01008

Characterizing transmissive diamond gratings as beam splitters for the hard X-ray single-shot spectrometer of the European XFEL N. Kujala et al. J. Synchrotron Rad. **26** (3), 708–713 (2019) doi:10.1107/S1600577519003382 Coherent soft X-ray pulses from an echo-enabled harmonic generation free-electron laser P. Rebernik Ribič et al. Nature Photonics **13** (8), 555–561 (2019) doi:10.1038/s41566-019-0427-1

Combining X-ray K <sub>1,3</sub>, valence-to-core, and X-ray Raman spectroscopy for studying Earth materials at high pressure and temperature: the case of siderite C. Weis et al. J. Anal. At. Spectrom. **34** (2), 384–393 (2019) doi:10.1039/C8JA00247A

Commissioning of a photoelectron spectrometer for soft X-ray photon diagnostics at the European XFEL J. Laksman et al. J. Synchrotron Rad. **26** (4), 1010–1016 (2019) doi:10.1107/S1600577519003552

Complete Characterization of Phase and Amplitude of Bichromatic Extreme Ultraviolet Light M. Di Fraia et al. Phys. Rev. Lett. **123** (21), 213904 (2019) doi:10.1103/PhysRevLett.123.213904

Consistent partial bosonization of the extended Hubbard model E.A. Stepanov et al. Phys. Rev. B **100** (20), 205115 (2019) doi:10.1103/PhysRevB.100.205115

Crystal structure of a domain-swapped photoactivatable sfGFP variant provides evidence for GFP folding pathway S. Kesgin-Schaefer et al. FEBS J. **286** (12), 2329–2340 (2019) doi:10.1111/febs.14797

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L. Samoylova et al. J. Synchrotron Rad. **26** (4), 1069–1072 (2019) doi:10.1107/S1600577519004880

Direct observation of picosecond melting and disintegration of metallic nanoparticles Y. Ihm et al. Nat. Commun. **10** (1), 2411 (2019) doi:10.1038/s41467-019-10328-4

Direct Visualization of Spatial Inhomogeneity of Spin Stripes Order in La<sub>1.72</sub>Sr<sub>0.28</sub>Ni<sub>04} G. Campi et al. Condens. Matter **4** (3), 77 (2019) doi:10.3390/condmat4030077</sub>

Do Images of Biskyrmions Show Type-II Bubbles? J.C. Loudon et al. Adv. Mater. **31** (16), 1806598 (2019) doi:10.1002/adma.201806598

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Electronic correlations and competing orders in multiorbital dimers: A cluster DMFT study M. Harland et al. Phys. Rev. B **99** (4), 045115 (2019)

doi:10.1103/PhysRevB.99.045115

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U. Boesenberg et al. Carbon **143**, 371–377 (2019) doi:10.1016/j.carbon.2018.11.031

### Electrospray sample injection for single-particle imaging with x-ray lasers

J. Bielecki et al. Sci. Adv. **5** (5), eaav8801 (2019) doi:10.1126/sciadv.aav8801

### Elucidation of the photoaquation reaction mechanism in ferrous hexacyanide using synchrotron x-rays with sub-pulse-duration sensitivity

A.M. March et al. J. Chem. Phys. **151** (14), 144306 (2019) doi:10.1063/1.5117318

### Evidence of Extreme Ultraviolet Superfluorescence in Xenon

L. Mercadier et al. Phys. Rev. Lett. **123** (2), 023201 (2019) doi:10.1103/PhysRevLett.123.023201

### Exact real-time dynamics of single-impurity Anderson model from a single-spin hybridization-expansion P. Kubiczek et al.

SciPost Physics **7** (2), 16 (2019) doi:10.21468/SciPostPhys.7.2.016

### Excitonic instability and unconventional pairing in the nodal-line materials ZrSiS and ZrSiSe

M.M. Scherer et al. Phys. Rev. B **98** (24), 241112 (2019) doi:10.1103/PhysRevB.98.241112

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Experimental 3D coherent diffractive imaging from photon-sparse random projections

K. Giewekemeyer et al. IUCrJ **6** (3), 1–9 (2019) doi:10.1107/S2052252519002781

Fate of transient isomer of CH<sub>2</sub>I<sub>2</sub>: Mechanism and origin of ionic photoproducts formation unveiled by time-resolved x-ray liquidography S. Park et al. J. Chem. Phys. **150** (22), 224201 (2019) doi:10.1063/1.5099002

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D.J. Higley et al. Nat. Commun. **10** (1), 5289 (2019) doi:10.1038/s41467-019-13272-5

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E.G.C.P. van Loon et al. Phys. Rev. B **98** (20), 205148 (2019) doi:10.1103/PhysRevB.98.205148

### First measurements with the K-monochromator at the European XFEL W. Freund et al.

J. Synchrotron Rad. **26** (4), 1037–1044 (2019) doi:10.1107/S1600577519005307

### First operation of the SASE1 undulator system of the European X-ray Free-Electron Laser S. Abeghyan et al. J. Synchrotron Radiat. **26** (2), 302–310 (2019)

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### X-ray tracking of structural changes during a subnanosecond solid-solid phase transition in cobalt nanoparticles

P. Vester et al. Phys. Rev. B **100** (24), 245425 (2019) doi:10.1103/PhysRevB.100.245425 Workshops, Summer Schools, and Seminars

### WORKSHOPS, SUMMER SCHOOLS, AND SEMINARS

### 23-25 JANUARY 2019

**European XFEL Users' Meeting** DESY, Hamburg, and European XFEL, Schenefeld, Germany

The European XFEL Users' Meeting is an annual opportunity to strengthen the interaction between European XFEL and the scientific user community. The scope of the meeting in 2019 included progress and status of the European XFEL, developments and advances of the instrument design, early user experiments, selected science applications, and ongoing developments in the field of X-ray FEL facilities.

Figure 3: Participants of the SCS satellite meeting "Early User Workshop: hRIXS @ SCS"



**Figures 1 & 2:** Impressions of the European XFEL Users' Meeting, during the opening session (left) and coffee break (right)

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### Workshops

### 4-5 MARCH 2019

**Time-Resolved Structural Studies – Synergy and Complementarity between ESRF and European XFEL** ESRF campus in Grenoble, France

The two-day workshop, which was hosted jointly by European XFEL and ESRF, focused on the science, instrumentation, and user communities of two complementary time-resolved instruments: the FXE instrument of the European XFEL and the ID09 beamline for structural dynamics of the ESRF.



**Figure 4:** Participants of the "New Scientific Capabilities at European XFEL" workshop on 25 March 2019

### 25-27 MARCH 2019

New Scientific Capabilities at European XFEL DESY, Hamburg, Germany

Two empty tunnels currently available at the European XFEL are planned to be upgraded in the mid term to two new FEL beamlines: SASE4 and SASE5. The scope of the workshop was a detailed analysis—both from the technical and scientific side—of ideas for upgrades that would enhance the capabilities of the facility. The workshop broadly addressed possible scientific topics related to the SASE4 and SASE5 upgrades.

Workshops, Summer Schools, and Seminars

### Summer Schools

### 2-8 JUNE 2019

International Summer School of Crystallography 2019 CFEL at DESY, Hamburg, Germany

Carmelo Giacovazzo, professor of crystallography at the University of Bari, Italy, lectured on the basics of crystallography, covering mathematical understanding of crystallographic point and space groups, diffraction experiments, structure factor calculations, systematic absences, determination of space groups, and many additional topics. Thomas Schneider from EMBL covered the background of phasing algorithms for structure determination of biomolecules. Participating students also learned about modern applications and instrumentation of protein crystallography experiments at advanced light sources, such as third-generation synchrotron and X-ray FELs.

#### 17-21 JUNE 2019

The Ultrafast X-Ray Summer School (UXSS 2019) CFEL at DESY, Hamburg, Germany

UXSS is an annual event jointly organized by the Center for Free-Electron Laser Science (CFEL) in Germany and the Stanford PULSE Institute in the USA. UXSS is intended to introduce students and postdocs to the latest science that is enabled by novel X-ray FELs. The programme of the school this year consisted of nine lectures given by distinguished scientists in the field, a one-day visit to European XFEL with instrument presentations and tours, and guided hands-on project work in which the participants worked out a mock proposal for beamtime at the European XFEL.



**Figure 5:** Participants of the Ultrafast X-Ray Summer School (UXSS 2019) at CFEL

### Seminars

### 5 FEBRUARY 2019

From single GaAs detector to pixelated sensor for radiation imaging camera Andrea Sagatova, Slovak University of Technology, Bratislava, Slovakia

#### 6 FEBRUARY 2019

**Development of PAL-XFEL undulator system** Dong-Eon Kim, Pohang Accelerator Laboratory, South Korea

#### 27 FEBRUARY 2019

Floquet analysis of excitations in solids Hannes Hübener, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

### 5 MARCH 2019

Probing C-H mixtures at conditions relevant to the interiors of giant planets, brown dwarfs, and stars Dominik Kraus, Helmholtz-Zentrum Dresden-Rossendorf, Germany

#### 14 MARCH 2019

Correlated systems in non-equilibrium conditions: few case studies Michele Fabrizio, International School for Advanced Studies SISSA, Trieste, Italy

### 19 MARCH 2019

High-resolution RIXS of cuprates and other 3d-TM oxides Giacomo Ghiringhelli, Politecnico di Milano, Italy

#### 20 MARCH 2019

Current advances in serial crystallographic data reduction using DIALS Aeron Brewster, Lawrence Berkeley National Laboratory, USA

### 2 APRIL 2019

The Ultrafast Einstein–de Haas Effect Steven Johnson, ETH Zurich and PSI, Villigen, Switzerland

### 3 APRIL 2019 PAL-XFEL: Past, present, and future Yong Woon Park, Pohang Accelerator Labo

Yong Woon Park, Pohang Accelerator Laboratory, South Korea

#### 16 APRIL 2019

Balanced detection for XAS at the photon noise limit Bill Schlotter, SLAC National Accelerator Laboratory, Menlo Park, USA

### 30 APRIL 2019

Ultrafast demagnetization dynamics by time-resolved XMCD Christine Boeglin, University of Strasbourg, France

### 14 MAY 2019

Investigation of warm dense matter with ultrafast and ultraintense lights Byoung-Ick Cho, Gwangju Institute of Science and Technology, South Korea

#### 28 MAY 2019

**15 years of single-particle imaging at FELs** Tomas Ekeberg, Uppsala University, Sweden

### 11 JUNE 2019

The LUXE experiment at the European XFEL Beate Heinemann, DESY and University of Freiburg im Breisgau, Germany

#### 26 JUNE 2019

X-ray views of disordered matter Giulio Monaco, University of Trento, Italy

#### 9 JULY 2019

Multilayer Laue lenses for extreme focusing Saša Bajt, DESY, Hamburg, Germany

#### 10 JULY 2019

Osmates on the verge of a Hund's-Mott metal-insulator transition: The different fates of NaOsO<sub>3</sub> and LiOsO<sub>3</sub> Alessandro Toschi, Technical University of Vienna, Austria

#### **3 SEPTEMBER 2019**

High-order interferometry at X-ray FEL sources Ivan Vartaniants, DESY, Hamburg, Germany

#### 12 SEPTEMBER 2019

Progress and challenges in delivering the ESS: Lessons learned in building world-leading research infrastructures Dimitri Argyriou, European Spallation Source ERIC, Lund, Sweden

### 16-21 SEPTEMBER 2019

Highlights der Physik 2019: Zeig Dich! Bonn, Germany 17 SEPTEMBER 2019 Non-equilibrium nanoscale control of charge, spin, and lattice motion in magnetic materials Hermann Duerr, Uppsala University, Sweden

#### 15 OCTOBER 2019

Operando investigations of heterogeneous catalysts: overcoming the spatio-temporal average Andreas Stierle, DESY and Universität Hamburg, Germany

21 OCTOBER 2019 Freiheit der Wissenschaft in Gefahr! Wie stark bedrohen Nationalismus, politische Spannungen und Fake News die Forschung? DESY, Hamburg, Germany

24 OCTOBER 2019 Towards end-to-end data management for large scale X-ray facilities Brian Vinter, University of Copenhagen, Denmark

### 28 OCTOBER 2019

The TMO Instrument: Opportunities and plans for time-resolved atomic, molecular, and optical science at LCLS-II Peter Walter, SLAC National Accelerator Laboratory, Menlo Park, USA

12 NOVEMBER 2019 Phonon photography? Hugh Simons, Technical University of Denmark, Kongens Lyngby, Denmark

26 NOVEMBER 2019 X-ray lasers shed light on the mysteries of water Anders Nilsson, Stockholm University, Sweden

28 NOVEMBER 2019 Status of optics installation at SwissFEL Uwe Flechsig, PSI, Villigen, Switzerland

29 NOVEMBER 2019 High repetition rate single-particle imaging Filipe Maia, Uppsala University, Sweden

2 DECEMBER 2019 SwissFEL: First experiments and future outlook Christopher Milne, SwissFEL, PSI, Villigen, Switzerland

3 DECEMBER 2019 Thermal and non-thermal dynamics on the nanoscale Anton Plech, Karlsruhe Institute of Technology, Germany Glossary

Glossary

Α

AGIPD Adaptive Gain Integrating Pixel Detector

B BMBF German Federal Ministry of Education and Research

С CCD Charge-coupled device

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

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 DESY Deutsches Elektronen-Synchrotron in Hamburg and Zeuthen, Germany

DFG German Research Foundation

### F. FXE

Femtosecond X-Ray Experiments [European XFEL instrument]

### H HED

High Energy Density Science [European XFEL instrument]

HiBEF

Helmholtz International Beamline at the European XFEL for Extreme Fields

INFN Istituto Nazionale di Fisica Nucleare in Rome, Italy

L LPD Large Pixel Detector

Μ MID Materials and Imaging Dynamics [European XFEL instrument]

S SASE Self-amplified spontaneous emission

SCS Spectroscopy and Coherent Scattering [European XFEL instrument]

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

SQS Small Quantum Systems [European XFEL instrument]

SXP Soft X-Ray Port [European XFEL instrument]

U UHH Universität Hamburg in Germany

UKRI UK Research and Innovation in Oxford, UK



### EUROPEAN XFEL ANNUAL REPORT 2019

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