

# **Enlightening Science**



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## Welcome to European XFEL

When the European X-ray Free Electron Laser opened its doors to the scientific community in September 2017, it marked the culmination of more than a decade of planning and construction. We are delighted to finally be able to start research and address the challenges of the future. In this booklet we would like to introduce you to this new international research facility that is now an exciting destination for scientists from across the globe looking to push the frontiers of scientific knowledge. At European XFEL, novel accelerator technologies have enabled the production of extremely intense and ultra-short X-ray pulses, providing scientists with a powerful tool for investigating the atomic structure and dynamics of matter. As a result, a whole new world of research possibilities has become accessible. Scientists, for example, will be able to understand and guide the fabrication of novel materials, to unravel the structure and function of biomolecules and use this knowledge to search for new pharmaceutical products, to examine states of matter in the laboratory that are naturally found only in the interior of planets and stars, and to provide important clues to solving the energy problems we face. We, together with our colleagues in the twelve shareholder and partner countries and the global scientific community, look forward to the scientific and technological advances the world's leading X-ray laser facility will enable in the years to come!

I invite you to read more about European XFEL in the following pages. Enjoy!

Prof. Dr. Robert Feidenhans'l

Managing Director and Chairman of the Management Board



The European XFEL's superconducting linear accelerator, the longest in the world, drives the X-ray laser using electrons accelerated to high energies.

#### At a glance

## A facility of superlatives

The European X-Ray Free-Electron Laser (European XFEL) is an international research facility of superlatives: **27 000 X-ray flashes per second and a brilliance that is a billion times higher than that of the best conventional X-ray sources will open up completely new opportunities for science.** Research groups from around the world come to the facility to investigate nanometre-scale structures, fast processes, and extreme states; take three-dimensional (3D) images of viruses and proteins; and film chemical reactions. The facility is operated by the European XFEL GmbH, a non-profit company that cooperates closely with its largest shareholder, Deutsches Elektronen-Synchrotron (DESY), and other organizations worldwide. The company has a workforce of more than 300 employees. In addition, about 240 DESY employees operate the accelerator for European XFEL.

With construction and startup costs of approximately 1.22 billion euro (at 2005 price levels) and a total length of 3.4 km, European XFEL is one of the largest and most ambitious new European research facilities. Currently, twelve European countries contribute to the European XFEL: Denmark, France, Germany, Hungary, Italy, Poland, Russia, Slovakia, Spain, Sweden, Switzerland, and the United Kingdom. Germany covered more than half of the construction costs, Russia about a quarter, and the other international shareholders between 1% and 3% each. In the first five years, the member countries will cover the operation costs according to their contribution to the construction.







The scientific instruments are the culmination of an intensive research and development effort, including state-of-the-art methods for provision of samples—including this liquid jet setup.

#### **Research opportunities**

## **Opening up research areas**

Smaller, faster, stronger—the European XFEL will open up areas of research that were previously inaccessible, thereby attracting top-level scientists from all over the world. The facility brings together very different scientific disciplines, which, in turn, will challenge and foster one another, stimulating a multitude of ideas leading to new products and improvements in existing ones. The X-ray flashes of the European XFEL have a higher brilliance than those of any other facility in the world. The flashes typically last between a few tens and a few hundreds of femtoseconds (quadrillionths of a second). These two outstanding features will enable researchers to make films of ultrafast processes, such as chemical reactions or configuration changes of biomolecules.

Using the X-ray flashes of the European XFEL, scientists will also be able to map the atomic details of viruses, decipher the molecular composition of cells, take 3D images of the nanoworld, and study processes similar to those in the interior of planets and stars. The new facility will benefit many scientific fields and technological applications, including biology, medicine, pharmacology, chemistry, materials science, physics, astrophysics, energy research, environmental research, electronics, nanotechnology, and photonics.

# Biology, medicine, and pharmacology

Soon after Wilhelm Conrad Röntgen discovered X-ray radiation in 1895, X-ray images were available all over the world. In 1912, Max von Laue discovered that crystal structures could be studied by diffracting monochromatic X-rays. Decoding the structure of DNA in 1953 was possible thanks to X-ray radiation.

More than half a century later, scientists have gained much deeper insights into the mechanisms of life, but numerous questions remain. With the X-ray flashes of the European XFEL, scientists are able to **analyse the structure of many more biomolecules and biological entities**—such as proteins, cells, or membranes—than was possible before. Even more, researchers will be able to study how these entities change while working. Understanding the structure of the entities, as well as their temporal changes, will provide insights into their functions, and is expected to form an important basis for the development of future medicines, such as antiviral drugs.



A pulse of X-rays from a free-electron laser illuminates a biomolecule. Before the molecule is destroyed by the pulse, it scatters a portion of the X-rays, creating a diffraction pattern. Many patterns from differently aligned copies of the molecule will enable scientists to determine its three-dimensional structure.

# Chemistry

Catalysis is a process that speeds up chemical reactions. In more than half of all chemical production processes, catalysts play an important role.

Nevertheless, little is known about how catalysis works on the atomic level. Likewise, many other chemical processes need to be better understood on this detailed scale. Such an understanding could lead to more efficient production mechanisms and new products. The X-ray flashes of the European XFEL allow scientists to film chemical reactions with unprecedented precision. They will be able to find out how molecules and catalysts interact with each other on the molecular time scale. This knowledge will help researchers understand how these processes can be further improved.



A car's catalytic converter, which reduces pollution in the exhaust. The European XFEL could improve the understanding of the process of catalysis and help make more efficient, less toxic catalysts.



Molecular movies: First, a laser flash (red) triggers a chemical reaction. A second pulse (blue), now from the free-electron laser, is then sent at varying time intervals after the first one to take snapshots of the changes that have occurred in the molecule.

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# **Materials**

Over the past few decades, a variety of completely new materials have been developed. X-ray science has played an important role in many of these developments. Properties such as durability, conductivity, or magnetization, can, however, still be better tailored to specific needs. Experiments at the European XFEL, which measure structural and dynamic properties of materials simultaneously, can help to **improve known materials and develop new ones** with revolutionary characteristics.

# **Electronics**

Our daily lives would be unthinkable without the inexorable progress made in electronics and computer technology. Faster chips and hard discs providing more memory require an ever better understanding of the properties of materials and how to optimize them. Research at the European XFEL offers **new insights into the nanoworld, into magnetism, and into the properties of materials**, with possible applications for faster computers and greater data storage capacity.



The European XFEL allows researchers to improve data rates and storage capacity of computers and consumer electronics.

# **Physics**

Physical processes are at the origin of many phenomena exploited in our daily lives. At the European XFEL, researchers will not only be able to study static properties of gases, liquids, or solids, they will gain new insights into the dynamics of matter. Dynamic processes can be initiated using electric or magnetic field pulses, or ultrashort optical laser flashes, as well as by extreme straining of samples.

The results of these investigations will contribute to our knowledge about driven, reversible processes and accidental, irreversible processes. The first class of processes, such as phase transitions and oscillations (for example, triggered by optical light pulses), could be exploited in **new technological applications**. Studying the second class of processes, such as crystallization or crack formation and propagation, could lead to **new materials** with improved properties, such as strength and elasticity.



Experiment at the DESY X-ray radiation source PETRA III

## Astrophysics and the science of extreme states

A specific state of excited matter is reached at extreme temperature, density, and pressure. In extreme conditions, if the atoms are ionized (that is, have lost some or all of their orbiting electrons), this state of matter is called a plasma. The X-ray flashes of the European XFEL enable scientists to produce and analyse plasmas that, to date, have been inaccessible in the laboratory, as they occur only in places such as the core of planets. Astrophysicists can use the resulting data to verify their theories on the formation and current geophysical state of the Earth. Scientists will also be able to study the conditions in the interior of heavier planets and to shed new light on the formation and evolution of the solar system.



The European XFEL enables scientists to obtain new insights into plasmas and other extreme states of matter existing inside stars or planets.

# Nanotechnology

The structures that we are able to produce artificially are becoming smaller and smaller. Already, nanomaterials are part of our daily lives. Such materials are composed of structures that are approximately between 1 and 100 nanometers in size, that is, between one billionth and a ten-millionth of a metre. At this level, materials exhibit surprising new properties, which often depend on the size of the particle. The short wavelength, high coherence, and ultrashort X-ray flashes of the European XFEL are ideally suited to **investigate the spatial structure and temporal behaviour of nanomaterials**. These insights could lead to new tailor-made nanomaterials, thereby laying the foundation for tomorrow's technologies.

## **Photonics**

Laser technology has long been part of many applications we use every day. For instance, the use of visible light in communications technology already plays a major role in our lives. Research at the European XFEL could help to **extend the range of photonics from visible light to the X-ray realm**, with the possibility of developing new organic photosensitive materials for transistors, computers, lasers, and other light sources. In addition, the European XFEL will allow research into non-linear effects at very short wavelengths. In the range of visible light, non-linear optical materials are used to build optical switches or for frequency doubling of optical lasers (for example, to convert them from infrared to green or violet).



At the European XFEL, nanoparticles and materials of the future, such as carbon nanotubes, can be studied in detail at the atomic level.



Artificial photosynthesis. In the future, biofuels could be produced from  $CO_{2^1}$  sunlight, and water, imitating processes within a plant cell. The European XFEL could take time-resolved pictures of the reactions that occur in the plant and show them in atomic scale detail. This will lead to a better understanding of these reactions, enabling scientists to optimize them for highly efficient and clean fuel production.

## **Environmental research**

A better understanding of processes in our environment at the atomic level will provide deeper insights into the reasons for environmental change. It will also help us to find new solutions, such as **artificial photosynthesis**, to address related problems. The intense X-ray flashes of the European XFEL can lead to the development of new catalysts and to the replacement of rare or toxic materials in industrial production. For example, scientists can examine soot particles with the aim of developing more efficient combustion processes or nanomaterials that minimize their eventual environmental impact.

## **Energy research**

Growing populations and developing economies require increasing amounts of energy, but resources are limited. Known sources of energy are running out, or their use entails difficulties for the environment. To find answers to these challenges, scientists can use the X-ray flashes of the European XFEL to study **processes occurring in solar cells and fuel cells**. The flashes will also help them to create and analyse plasmas that could be exploited in future fusion reactors.

#### In comparison

## **Research using X-rays**

X-rays are electromagnetic waves like radio waves, microwaves, or visible light, but with a much shorter wavelength. While no conventional optical microscope is able to "see" objects smaller than the visible light wavelengths, X-rays have sufficiently short wavelengths to "see" matter at the atomic level of detail. X-rays range from lower-energy "soft" X-rays, which have wavelengths comparable to large molecules, to higher-energy "hard" X-rays, which have shorter wavelengths that are comparable to individual small molecules and atoms.



The spectrum of electromagnetic radiation, showing the size of the wavelengths of each type of radiation in comparison to different objects. The shorter the wavelength of the light, the smaller the objects that can still be "seen" with it.

In the 1950s, X-rays played a decisive role in discovering that, in a DNA molecule, atoms are arranged to form a double helix, like a circular ladder, and that the rungs of this "ladder" carry genetic information. This landmark discovery exemplifies how understanding structure is key to understanding function—a principle that is also very important in other fields, such as chemistry or materials science.

The determination of complex molecular structures requires very bright X-ray sources. Particle accelerators, in particular electron accelerators such as synchrotrons, are extremely bright X-ray sources that can be millions of times brighter than medical X-ray tubes. Since the 1960s, synchrotrons have revolutionized the study of biomolecules. In 1980, the number of biomolecules with a known atomic structure was about 70. In August 2017, this number exceeded 125 000; in over 99 000 of these, the structure was determined by synchrotron X-rays. Today, synchrotrons are the most important tool in determining the structure of biomolecules, and six chemistry Nobel Prizes have been awarded for research in which synchrotron sources played a decisive role.



One of the first studies of a biological molecule using an X-ray free-electron laser revealed the structure of a protein found in the pathogen that causes sleeping sickness.

Over the past few years, another major leap forward in the brightness of X-ray sources has been achieved by free-electron lasers (FELs), based on linear accelerators delivering pulses of X-rays that have three extraordinary properties:

- FEL pulses are extremely bright, about 100 million to a billion times brighter than synchrotron X-rays.
- FEL pulses are extremely short, down to a few tens of femtoseconds. A femtosecond is a millionth of a billionth of a second; in one femtosecond, light travels less than one hundredth of the thickness of a human hair.
- FEL pulses have a quality known as spatial coherence, which means that the waves of the laser light are in phase and reinforce one another. This is a quality that makes X-ray FEL pulses much more useful for experiments than conventional X-rays.



Light quality and wavelengths of different light sources in comparison. Laser beams (which are coherent) have a higher light quality than ordinary light (called incoherent, represented here by lamps). Large light source facilities are shown to the right. X-ray free-electron lasers (orange) are capable of producing coherent light within the X-ray portion of the spectrum. Synchrotrons cover a broad spectrum of wavelengths but can only produce incoherent light.

# FEL light sources worldwide

Along with the European XFEL in Germany, there are hard X-ray free-electron lasers in the US, Japan, South Korea, and Switzerland. The Linac Coherent Light Source (LCLS) X-ray FEL at SLAC National Accelerator Laboratory in California and the SPring-8 Angstrom Compact Free Electron Laser (SACLA) in Japan have been open for user operation for the past few years. The other facilities followed in 2016 and 2017. The operating principles behind these facilities are very similar: electrons are first accelerated to high energies and then made to generate high-intensity X-ray laser light. Whereas LCLS, SACLA, SwissFEL, and PAL-XFEL rely on conventional accelerator technologies, the European XFEL accelerator operates at -271°C using superconducting technology.



FEL light sources worldwide. Currently, the only hard X-ray FELs accepting users are SACLA in Japan and LCLS in the United States.

The LCLS-II will also use such superconducting technology. Superconductivity allows the creation of an electron beam of especially high quality, composed of many electron bunches lined up behind each other. This high number of electron bunches allows the European XFEL to generate many more X-ray flashes per second than other facilities. Certain experiments will be possible only at the European XFEL because of its much higher repetition rate. The higher number of electron bunches will also allow three of the six starting instruments to be used simultaneously.

Facility	LCLS USA	LCLS-II CuRF	LCLS-II SCRF	SACLA Japan	European XFEL	SwissFEL Switzerland	PAL-XFEL South Korea
Max. electron energy (GeV)	14.3	15	5.0	8.5	17.5	5.8	10
Wavelength range (nm)	0.1-4.6	0.05-5.0	0.25-5.0	0.06-0.3	0.05-4.7	0.1–7	0.06–10
Photons/ pulse	~ 1012	2 x 10 <sup>13</sup>	3 x 10 <sup>13</sup> (soft X-rays)	2 x 10 <sup>11</sup>	~ 1012	~ 5 x 1011	10 <sup>11</sup> –10 <sup>13</sup>
Peak brilliance	$\begin{array}{l} 2.7 \ x \ 10^{34} \\ \text{(with seeding)} \end{array}$	$\begin{array}{c} 2.7 \ x \ 10^{34} \\ \text{(with seeding)} \end{array}$	1 x 10 <sup>32</sup>	1 x 10 <sup>33</sup>	5 x 10 <sup>33</sup>	1 x 10 <sup>33</sup>	1.3 x 10 <sup>33</sup>
Pulses/ second	120	120	1 000 000	60	27000	100	60
Date of first beam	2009	2019	2020	2011	2017	2016	2016
Start of user operation	2009	2019	2020	2012	2017	2018	2017

Comparison of the properties of hard X-ray light sources, including European XFEL. LCLS-II CuRF: non-superconducting "warm" linear accelerator; LCLS-II SCRF: superconducting "cold" accelerator



Number of transistors in processors

Comparison in rates of development between X-ray light sources and computer processors. The rate of increase of relative brightness of X-ray sources since the 1890s surpasses the increase in the number of transistors on a silicon processor chip since the 1960s (the latter described as "Moore's Law").

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# 1. Accelerator: bringing electrons to high energies

The first part of the European XFEL facility is a 1.7 km-long particle accelerator that brings bunches of electrons to high energies at nearly the speed of light. The linear accelerator (linac) geometry is essential for the high quality of the electron beam and the high peak current required for the SASE process (described in the next section), which yields X-rays with laser-like properties. Based on a technology developed by DESY and its international partners, the linac accelerates the electrons in special cavities, called resonators. In the resonators, an oscillating microwave, a radiofreqency (RF) pulse generated by a so-called klystron, transfers its energy to the electrons.

The resonators are made of the metal niobium and have superconducting properties when cooled down to very low temperatures. At a temperature of -271°C, they lose their electrical resistance. Electrical current then flows through a thin layer of the resonators' inner surface with basically no loss, and nearly the entire energy of the microwave field that is fed into the resonators can be used for the acceleration of the electron bunch.



European XFEL tunnel with linear accelerator



Building the 1.7 km-long electron accelerator: 100 yellow superconducting cryomodules, each 12 metres long, were mounted at the top of the ceiling in the accelerator tunnel.

The electrons are generated in the injector, the 45 m-long first part of the superconducting particle accelerator. When a negatively charged caesium telluride electrode is exposed to a UV laser pulse, billions of electrons are ejected from its surface and form a cloud called a bunch. Each second, the injector produces 27 000 tightly packed bunches of electrons and gives them their initial energy. A klystron powers a short normal conducting accelerator that pushes the bunches away from the electrode and injects them into the superconducting second part of the injector. In the main section of the linac, RF pulses boost the electrons to their target energy of up to 17.5 gigaelectronvolt (GeV).

The specifications that the electron source must meet are very challenging, as even the smallest irregularities in the bunch substructure at the beginning would amplify in the course of the acceleration process and result in an electron beam of insufficient quality to generate the radiation required for the experiments at the European XFEL. In a high-quality electron beam, all electrons are within a well-defined volume and have almost the same energy. Only a very small part forms the "halo" surrounding the core of the bunch.



The injector, is located at the beginning of the facility. It contains the electron source and provides the initial energy to the electrons.

Electromagnetic fields accelerate the electrons in the superconducting resonators.

# 2. Undulators: inducing electrons to emit light

After they are brought to high energies, the accelerated electrons race through undulators periodic arrangements of magnets that force the particles onto a tight slalom course. In the process, the electrons emit X-ray radiation that amplifies more and more.

This amplification process is induced by the interaction of the X-ray radiation with the electrons. Since the radiation is faster than the electrons speeding along their slalom path, the radiation overtakes the electrons flying ahead and interacts with them along the way, accelerating some and decelerating others. As a result of this interaction, the electrons gradually organize themselves into a multitude of thin disks, spaced at the X-ray wavelength. The key property of this "self-amplified spontaneous emission" (SASE) process is that all of



European XFEL tunnel with undulators



To generate the extremely short and intense X-ray laser flashes, bunches of high-energy from the superconducting accelerator are directed through special periodic arrangements of magnets called undulators.

the electrons in a disk and the majority of electrons in neighbouring disks within a bunch emit their light in sync. The synchronized emissions within each disk and among neighbouring disks result in extremely intense X-ray flashes with the properties of laser light. The superconducting accelerator delivers 10 pulse trains per second, with each train consisting of up to 2700 electron bunches. This results in **27** 000 flashes per second, a unique property of the European XFEL.

Since the structure of thin disks forms fully only after a certain length of interaction between the electrons and the radiation, free-electron lasers require very long undulators. At the European XFEL, the electron beam passes through undulators that are up to 212 m long. Such an undulator consists of up to 35 segments, each 5 m long, with magnets followed by 1.1 m-long intersections.



Left: The magnets (the green blue-structure in the illustration) force the electron bunches on a slalom course, where they emit X-ray light at each turn. Right: Exponential growth of the FEL pulse energy and microbunching: Because the radiation is faster than the electrons on their slalom path, the radiation overtakes the electrons flying ahead and interacts with them along the way, accelerating some of them and slowing others down. The electrons then gradually organize themselves into a multitude of thin disks. All electrons in neighbouring disks emit light in sync, producing extremely short and intense flashes. The wavelengths of the radiation generated in the undulators can be varied by adjusting either the energy of the electrons or the value of the magnetic field of the undulators. This field strength is varied by changing the distance between two rows of magnets, called the undulator gap. While higher electron energy leads to shorter wavelength radiation, a stronger magnetic field has the opposite effect, resulting in a wider slalom course and thus X-ray radiation with a longer wavelength. As one electron accelerator can drive several undulators by sending consecutive sets of bunches into different tunnels, it is possible to generate radiation with different properties for different scientific instruments.

As a first step, the European XFEL will provide three undulators with at least six scientific instruments. Two of them will be available in 2017; the other four are scheduled to follow in 2018. A bunch distribution scheme will allow sending only the bunch pattern requested for the experiment to the respective beamline. A shutter will enable scientists to even select individual photon pulses for experiments.



The magnets of the undulators must be adjusted with micrometre accuracy to obtain the extremely precise magnetic field required for X-ray generation in the European XFEL. The distance between the upper and lower row is the undulator gap. During operation, the gap is between 10 and 25 mm, depending on the electron energy and the desired X-ray wavelength.

## Self-seeding

After they are brought to high energies, the accelerated electrons race through undulators. When X-ray laser light is generated in the SASE process, random spontaneous emissions are used to initiate, or "seed", the light generation. These emissions amplify into a broader spectrum of X-ray wavelengths, which is not desirable for many applications. In 2010, researchers from DESY and European XFEL in Hamburg devised a way to dramatically improve the already remarkable features of X-ray free-electron lasers by placing a diamond crystal in the path of the radiation between undulator segments near the starting point of light generation. The crystal selects a very narrow part of the spectrum, and only this is then further amplified in the following undulator. Since the seed is not generated by an external source but by the laser itself, the process is known as self-seeding, and the corresponding flashes could be used to take extremely sharp images. The scheme has been successfully tested at the Linac Coherent Light Source (LCLS) in California, and is now planned to be implemented in two undulator systems (SASE1 and SASE2, see p. 40) at the European XFEL.



Illustration of an undulator with magnets (yellow and blue), electron bunch (red), and a cone of X-ray light





The Femtosecond X-Ray Experiments (FXE) instrument is one of six instruments that will open new opportunities for science across many disciplines.

# 3. Scientific instruments: using X-ray flashes for research

The X-ray flashes of the European XFEL will facilitate a **large variety of very different experiments** at several different scientific instruments. Depending on the experimental requirements, the X-ray flashes can be widened, focused, filtered, or weakened using optical elements, such as mirrors, gratings, slits, or crystals. The samples to be investigated are provided in the scientific instrument, where they interact with the X-ray flashes. The basic idea behind a typical experiment at an X-ray free-electron laser (X-ray FEL, or XFEL) is easy: illuminate a sample with intense X-ray flashes and record the properties of the photons (that is, the light particles) emerging from the sample with a suitable set of detector elements. The data is then processed for analysis.

Each scientific instrument at the European XFEL is being optimized for a particular purpose. Each experiment requires light with special properties, which means that the instruments are permanently assigned to the different beamlines of the European XFEL. The imaging of single particles, for instance, calls for radiation with especially short pulses and high power, whereas the investigation of small objects in strong fields necessitates a high intensity and longer wavelengths.

# The following instruments will be available at the European XFEL

#### SPB/SFX – the Single Particles, Clusters, and Biomolecules / Serial Femtosecond Crystallography instrument

SPB/SFX will be used to investigate crystalline and non-crystalline matter. A particular emphasis is placed on the determination of three-dimensional structures of biological objects. Examples are biological molecules including crystals of macromolecules and macromolecular complexes as well as viruses, organelles, and cells—though the instrument will also be capable of resolving non-biological samples using similar techniques. In addition, scientists will be able to study slow, fast, and very fast structural changes and reactions of the biological systems. One ultimate goal is to explore the feasibility of achieving near-atomic resolution from samples down to the size of a single biological macromolecule without the need to first grow crystals.



The SPB/SFX instrument will enable the determination of three-dimensional structures of biological objects, clusters of atoms and molecules, and tiny crystals.

#### FXE – the Femtosecond X-Ray Experiments instrument

FXE will enable ultrafast pump-probe experiments on extremely short time scales – 100 femtoseconds and below – for a broad scientific community. It will deliver new information about geometric and electronic structures serving applications in many fields, particularly in the areas related to fast chemical processes and reactions, photovoltaic applications and photosyntheses, catalytic processes, and material science. The ability to follow these ultrafast processes and their intermediate steps like in a slow-motion molecular movie could help to better understand, imitate, and optimize these processes.



The FXE instrument is specially designed for investigations of ultrafast processes, such as the intermediate steps of chemical reactions.

#### **HED** – the High Energy Density Science instrument

HED will be used to study matter under extreme conditions of pressure, temperature, or electromagnetic fields that will be generated by high-energy optical lasers, diamond anvil cells, or pulsed magnets. Scientific applications will be studies of matter occurring inside astrophysical objects such as exoplanets, of new extreme-pressure phases and solid-density plasmas, and of phase transitions of complex solids in high magnetic fields. The instrument will enable researchers to refine planetary models, shed light on superconductivity, and explore laser-matter interaction with highest resolutions.



The HED instrument's main interaction chamber will be where extremely energetic solid matter, like that found inside planets, can be studied.

#### **MID** – the Materials Imaging and Dynamics instrument

MID aims at structural investigations of crystalline, nanostructured, or less well-ordered materials, such as glasses, liquids, and biological substances. It will also be possible to look at ultrafast dynamic processes such as atomic motion using specialized time-resolved X-ray imaging techniques. Applications comprise the exploration of visco-elastic properties in liquids and glasses, polymer dynamics, phase transitions, protein folding, or switches in magnetic orientation. Better understanding of structure and dynamics can lead to materials with tailor-made special characteristics and applications, for instance in energy conversion and storage or in magneto-optical memory devices.



The MID instrument will enable studies of exotic states of matter and their transitions.

#### SQS – the Small Quantum Systems instrument

SQS is dedicated to the study of free atoms and molecules, as well as clusters and nano-particles that consist of up to several thousands of atoms. Experiments will focus on "non-linear" multi-photon processes beyond the conventional "linear" process of absorbtion of just one photon, and on time-resolved investigations of the ultra-fast molecular fragmentation caused by these processes. Perfectly exploiting the high repetition rate, it will be possible to fully analyze multiple ionization processes or to capture the complete picture of bond breaking in molecules. In small systems, an unrivaled precision in characterizing these highly complex processes can be achieved, providing new insights into the interaction of light with matter at the atomic level, relevant for fundamental research in general and for scientific fields such as photochemistry or plasma- and astrophysics in particular.



The SQS instrument will enable studies of the interaction of light and matter that reveal insights into numerous atomic and molecular processes.

#### **SCS** – the Spectroscopy and Coherent Scattering instrument

SCS will enable time-resolved experiments to unravel the electronic and structural properties of soft matter, magnetic materials, and complex structures, such as nanostructured transition metal oxides with functional properties like high temperature superconductivity. The soft X-rays will be used to allow resolutions of up to 10 nanometres. Areas of application are materials science and studies of nanomaterials and dynamic processes. The instrument can be used to understand and develop new functional materials, e.g. for IT, medicine, energy research, or catalysis. Scientists, for example, will be able to investigate rapid changes of material properties such as magnetization or conductivity that are needed for the fast storage of information. A combination of coherent X-ray scattering with spectroscopy methods will make it possible to investigate atomic as well as electronic details.

More instruments will be planned and built in the coming years (see image on p. 40).



The SCS instrument will open new opportunities to study the electronic and structural properties of soft matter, magnetic materials, and complex structures.

# **Beamlines of the European XFEL**





The European XFEL will provide beamlines for X-ray flashes with different properties.

Scientific instrument	nm-scale structures	Ultrafast processes	Extreme states	Beamline
<b>SPB / SFX</b> Ultrafast coherent diffraction imaging: structure determination of single particles, such as atomic clusters, biomolecules, virus particles, or cells; serial femtosecond crystallography	•	•		SASE1
<b>FXE</b> Femtosecond X-ray experiments: time-resolved investigations of the dynamics of so- lids, liquids, or gases		•		SASE1
MID Materials imaging and dynamics: structure determination of nanodevices and dynamics at the nanoscale	•	•		SASE2
<b>HED</b> High energy density science: investigation of matter under extreme conditions using hard X-ray FEL radiation, for instance probing dense plasmas		•	•	SASE2
<b>SQS</b> Small quantum systems: investigation of atoms, ions, molecules, and clusters in intense fields as well as non-linear phenomena		•	•	SASE3
<b>SCS</b> Spectroscopy and coherent scattering: electronic and atomic structure and the dyna- mics of nanosystems and of non-reproducible biological objects using soft X-rays	•	•		SASE3



Data collection at very fast timescales (figures on the right side): Single pulse coherent diffraction imaging by Chapman et al. with the free-electron laser FLASH at DESY. Image of the first (a) and second pulse (b) at 32 nm. The second pulse shows that the structure has been destroyed by the first pulse. The original microstructure (c) was recovered (d) from the diffraction pattern of the first pulse.



Highly specialized optical lasers activate reactions in samples before the X-rays investigate the resulting process.

# 4. Optical lasers, detectors, and data acquisition: harvesting for science

One feature that singles out the European XFEL from other X-ray laser facilities is that it will produce up to 27 000 flashes per second. These flashes are not distributed evenly but come in bursts of 10 trains per second (burst mode). To make use of this high repetition rate, suitable instrumentation is needed, including **optical lasers**, special two-dimensional (2D) **detectors**, **electronics** to transport and reduce data, and the **storage** capacity and software solutions to analyse these data. To develop this instrumentation, European XFEL runs a unique research and development programme.

# Optical lasers for experiments: exciting the states

The European XFEL will provide pulses of extremely bright X-ray light that are so short, scientists will be able to observe nano-scale processes that are otherwise too fast to measure. Highly specialized pulsed optical lasers, synchronized with the European XFEL X-ray pulses, are used to activate, or **pump**, a reaction within the samples, before the X-ray pulse is used to investigate, or **probe**, the dynamics of that process.

Optical lasers capable of producing ultrashort pulses for research purposes are commercially available. However, with 2700 pulses within 600 microseconds, the burst emission pattern of the European XFEL, combined with the laser power and timing specifications required by its six experiment stations, is far beyond the scope of commercial laser technology. Laser scientists and engineers at European XFEL have, therefore, developed a pump–probe laser based on optical parametric amplification, tailored for the specific needs of experiments at European XFEL. The high pulse repetition rate and power of the optical lasers enable experiments at the highest possible X-ray pulse rate, with optical pulse parameters such as energy and pulse duration far beyond that of commercial systems.



An intensive research and development programme is resulting in ultrafast detectors that are capable of recording both very few and very many particles of light at once.

# **Detector development**

In a typical experiment, scientists deduce structural information on, for example, viruses, nanoparticles, and single molecules from 2D patterns of scattered photons. The European XFEL provides highly sensitive and ultrafast 2D detectors to measure such patterns. The 27 000 X-ray flashes per second produced by the European XFEL come in 10 trains per second, each train comprising 2700 flashes at a distance of only 220 nanoseconds (ns, or billionths of a second). The objective of the novel detectors is to capture, out of a possible 27 000 flashes per second, as many of the best flashes as is technically feasible, typically 3000 to approximately 5000 for the first new generation detectors.

Some areas of the detector will be bombarded by tens of thousands of photons, while others will be hit by only a few at best. A detector capable of measuring very few and very many photons has a high dynamic range. The dynamic range of the detectors at the European XFEL supercedes commercially available consumer cameras and detectors by many orders of magnitude. Since the interval between two pulses (220 ns) is much shorter than the time needed to transport the information from the detector to the data acquisition systems, the data generated within a train has to be stored and processed in the detector before the information is transmitted to the data centre.



Detectors for the European XFEL, such as the Large Pixel Detector developed in partnership with the Rutherford Appleton Laboratory in the United Kingdom (left), can provide detailed and clean diffraction data outputs, such as those shown in simulation (right), quickly enough to record reliably with the European XFEL's repetition rate.

# **Data acquisition**

Experiments at the European XFEL produce enormous amounts of data, all of which needs to be stored and made available for analysis. Each of the 2D pixel detectors, for example, will deliver 10 to 40 gigabytes (GB) of data—enough information to fill up to six DVDs—every second. According to current estimates, operating all six instruments will produce **10 million GB, or 10 petabytes (PB), of data per year**. In the future, this may increase to over 50 PB per year as a result of improved detector resolution. Storing 50 PB of data would require 10 million DVDs, which, if stacked on top of one another, would be 12 km high. At the European XFEL, of course, more advanced technologies will be used (see p. 47).

At many operating X-ray facilities, scientists can bring their own hard disk drives, copy their data onto the drives, and then do their analyses at home. For the European XFEL, a new approach has been implemented. Data is stored securely in a large storage system, exploiting technologies similar to those used by internet search engines. Data processing services are provided as well. Karabo, the control and analysis software framework developed at European XFEL, helps scientists with everything from moving samples like nanocrystals; to storing, mining, and analysing data; to visualizing the results.



Development and verification of high precision electronics are crucial for the demanding technology of the European XFEL.

Computer systems at the European XFEL have been developed to deal with the enormous flow of data from the experiments.

# **Technical details**

Some highlights of the data handling system at the European XFEL:

- Initial size of the storage system will be 10 PB (1 PB = 1 million GB = 10<sup>15</sup> bytes), increasing over time to 50 PB.
- Lossless data compression will be applied on the fly whenever possible. For single small biological molecules, it will be possible to compress the data to 5% of its original size. Solids, gases, and liquids do not allow such extreme compression rates.
- Hard disks will be used to store raw data as well as the results of scientific analysis for about one year. After that, all raw data will be moved to a tape archive for long-term storage.
- Computing clusters close to the data archive will be used to analyse the data.



In collaboration with international partners, European XFEL develops data acquisition, data management, and scientific computing hardware, as well as software for beamlines, experiments, and data analysis.

# **European XFEL GmbH**

The construction and operation of the European XFEL facility has been entrusted to the European X-Ray Free-Electron Laser Facility GmbH (European XFEL), a non-profit limited liability company under German law. The company directly and exclusively pursues **non-profit objectives in the field of science and research**, and cooperates closely with DESY and other research organizations worldwide. In particular, the European XFEL GmbH is in charge of the following:

- Coordination and monitoring of the construction activities
- Scientific policy and strategy
- Construction of the beamlines, scientific instruments, and associated infrastructure
- Operation of the facility and the user programme
- Further development of the facility, based on a vigorous research and development programme
- Related to the aforementioned tasks: management, supervision, and controlling of all financial and other resources made available by the shareholders or through collaboration contracts
- Knowledge and technology transfer to interested entities in the contracting countries, as well as general public outreach and knowledge transfer. The construction costs for the facility, which include commissioning, amount to more than 1.22 billion euro (in 2005 price levels). To a great extent, the European XFEL was realized by means of in-kind contributions by shareholders and partners.

## **Shareholders**

The shareholders of European XFEL are designated by the governments of the international partners, who commit themselves in an intergovernmental convention to support the construction and operation of the facility.



On 30 November 2009, ministers, state secretaries, and other government representatives from 10 partner countries met in the Hamburg City Hall to sign the international European XFEL agreement.

# Partner countries and shareholders (as of 2017)



\* future shareholders



Work on superconducting accelerator elements in the clean room at DESY

### **International network**

# **In-kind contributions**

Shareholders of the European XFEL GmbH have contributed to the construction in cash or in kind. In-kind contributions were delivered in form of components, human resources, or both. The value of in-kind contributions accounts for about 50% of the total construction budget.



Large electromagnets (a contribution from Russia, with some magnets tested through a Swedish contribution) for the electron beamline in the accelerator tunnel

Components for the linear accelerator were contributed by 17 institutes in 8 countries, including quality testing, which was a Polish contribution.

## International networks and cooperations

As a new research facility, European XFEL benefits directly from collaborations and agreements with related laboratories, scientific institutions, and universities. Since the foundation of the European XFEL GmbH in October 2009, a large number of such cooperations have been established. European XFEL is a member of EIROforum, the partnership of several European intergovernmental research organizations. For a list of cooperating institutions go to www.xfel.eu/organization/cooperation.

Country	Acronym	Name	City
Denmark	DTU	Technical University of Denmark – Physics Department	Risø
France	CEA	Commissariat à l'énergie atomique et aux énergie alternatives – IRFU	Saclay
	CNRS	Centre national de la recherche scientifique – IN3P2	Orsay
Germany	DESY	Deutsches Elektronen-Synchrotron	Hamburg
Italy	INFN	Istituto Nazionale di Fisica Nucleare	Milano
Poland	NCBJ	National Center for Nuclear Research	Swierk
	IFJ-PAN	Henryk Niewodniczański Institute for Nuclear Physics	Kraków
	WUT	Wrocław University of Technology	Wrocław
Russia	BINP	Budker Institute of Nuclear Physics of SB RAS	Novosibirsk
	IHEP	Institute for High Energy Physics	Protvino
	INR	Institute for Nuclear Research RAS	Troitsk
	JINR	Joint Institute for Nuclear Research	Dubna
	NIIEFA	D.V. Efremov Scientific Research Institute of Electrophysical Apparatus	St. Petersburg
Spain	CELLS	Consortium for the Exploitation of the Synchrotron Light Laboratory	Barcelona
	CIEMAT	Centro de Investigaciones Energéticas, Medioambientales y Technológicas	Madrid
	UPM	Universidad Politécnica de Madrid	Madrid
Sweden	KTH	Royal Institute of Technology	Stockholm
	MSL	Manne Siegbahn Laboratory	Stockholm
	SU	Stockholm University	Stockholm
	GU	Gothenburg University	Gothenburg
Switzerland	PSI	Paul Scherrer Institut	Villigen

# **Facility and Schenefeld research campus**

The European XFEL is located in the German federal states of Hamburg and Schleswig-Holstein. The main part of the facility is located in underground tunnels. This is where the electrons are accelerated and induced to generate the X-ray radiation, and where the X-ray flashes are transported to the instruments in the experiment hall. The facility is 3.4 km long and comprises three large sites. The **DESY-Bahrenfeld** site marks the beginning of the European XFEL. The main tunnel, which houses the electron accelerator, begins on this site at a depth of about 38 m underground. Under the **Osdorfer Born** site, the electron bunches are distributed into the first two tunnels, in which they generate X-ray light (see "Beamlines of the European XFEL" on p. 40). The **Schenefeld** site, location of the facility's headquarters, is the centre for research and innovation at which scientists and researchers from all over the world—supported by more than 300 employees of European XFEL—collect and analyse their scientific data. The new research campus in Schenefeld will also include a canteen and a guesthouse, which are expected to be completed in 2018.



Tunnel with X-ray beamline near the Schenefeld research campus



Future canteen building on the Schenefeld campus



The European XFEL headquarters and laboratories building



Architectural rendering of the headquarters building on the European XFEL research campus. The tunnels that lead the X-ray flashes to the scientific instruments end in an underground hall beneath the main building, which houses labs, offices, and seminar rooms.

# **Bahrenfeld site**



Aerial view of the DESY-Bahrenfeld site with the injector complex, modulator hall, and cryogenic hall in August 2016: (a) cryogenic hall, (b) injector entrance hall, c) modulator hall, d) tunnel entrance hall

# **Osdorfer Born site**



The Osdorfer Born site shown in August 2016 accommodates the shaft XS1, where the linear accelerator tunnel ends and the two first undulator tunnels start. The site will house a new hall as well as infrastructure installations for power, ventilation, and water.

# **Schenefeld site**



Aerial view of the Schenefeld site in August 2016



One of the compensation measures is the large area restoration of the Düpenau creek on the Schenefeld site.

## Safety and environmental protection

Safe operation is the prime requirement for the European XFEL facility. Its operation below and in densely populated areas bears no special risk. Reliable access control systems, such as those that have been in use at DESY for years, ensure that no one can enter the areas that are closed during operation. Even in the unlikely event that an electron beam should leave its trajectory in the accelerator, it would be instantly directed into the corresponding electron absorber, and operation would be shut down immediately.

Before construction of the European XFEL began, an independent environmental impact study ruled out any negative repercussions on climate, air, groundwater, or surface water. As a matter of principle, construction work has been carried out in a way that preserves large trees, typical hedges, and other near-natural copses. This environmentally friendly approach is lessening the impact on the plants, animals, soil, and landscape of the neighbourhood. After construction, European XFEL has **restored neighbouring areas to their previous states** and increased their value by laying out near-natural green spaces, hedges, groves, and areas that have been returned to nature.

For more information on safety and environment, visit our website www.xfel.eu.

#### **Facts and figures**

## **Properties of the X-ray flashes**

- Flashes per second: 27 000 | The high repetition rate makes the European XFEL unique among the world's X-ray lasers. This is possible only thanks to superconducting accelerator technology operating at -271°C.
- Wavelengths: 0.05 to 4.7 nanometres (0.05 to 4.7 billionths of a metre) | The wavelengths are so short that atomic details become discernible.
- Duration: Down to a few tens of femtoseconds (quadrillionths of a second) | Thanks to this extremely short pulse duration, scientists can make films of ultrafast processes.
- Brilliance (photons/s/mm²/mrad²/0.1% BW): 5×10<sup>33</sup> (peak), 1.6×10<sup>25</sup> (average) | The brilliance is a measure of the number of photons generated within a specific wavelength range. The peak brilliance of the European XFEL is a billion times higher than that of the best conventional X-ray sources.
- Coherence | The coherence of the X-ray flashes makes it possible to use them for a wide range of interference experiments such as holography.

## Facility

- Type: X-ray free-electron laser (XFEL)
- Total length: 3.4 kilometres
- Depth of the tunnels: 6 to 38 metres below ground level
- Accelerator: Linear accelerator (1.7 kilometres), which speeds up electrons to an energy of 10 to 17.5 billion electron volts (GeV), expandable to 20 GeV
- Sites: DESY-Bahrenfeld (2 hectares), Osdorfer Born (1.5 hectares) and Schenefeld (15 hectares). The research campus is located in Schenefeld.

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