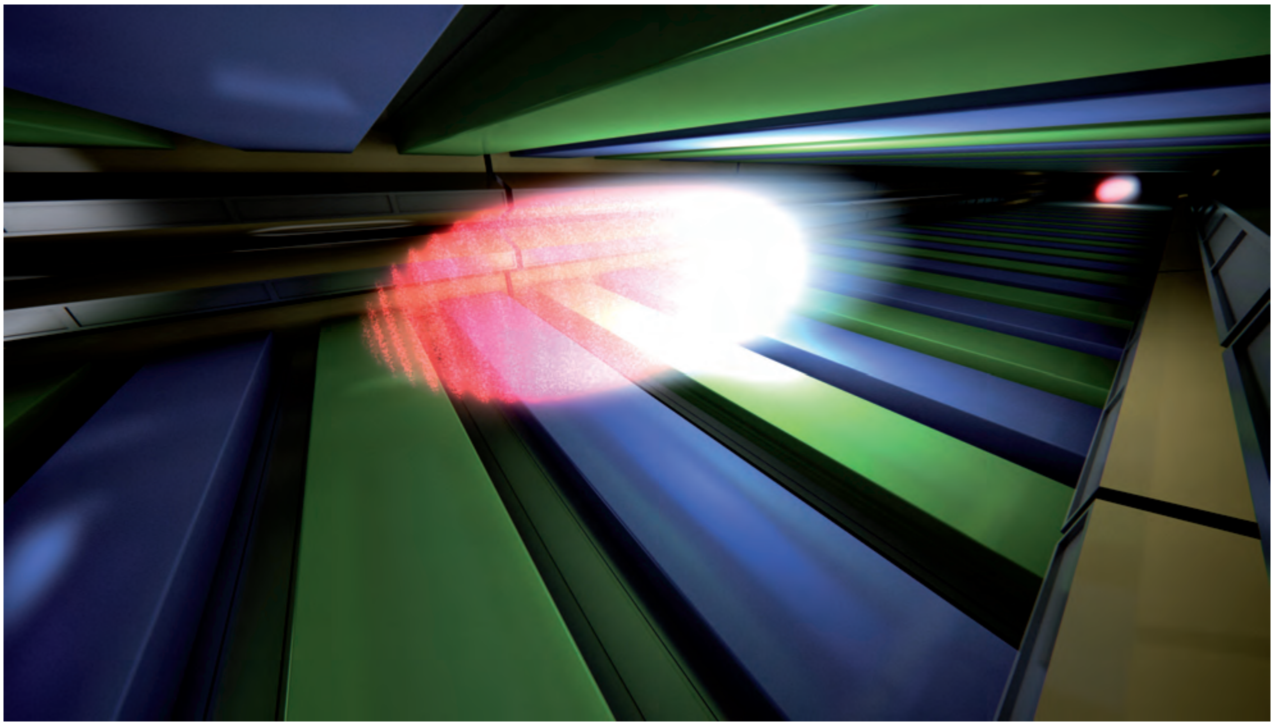
THE EUROPEAN X-RAY FREE-ELECTRON LASER FACILITY



AND THE CHALLENGES OF OUR TIME

CONTENT

THE EUROPEAN X-RAY FREE-ELECTRON LASER FACILITY AND THE CHALLENGES OF OUR TIME

1 Introduction: The European XFEL facility

This paper illustrates the benefits to society expected from the European X-Ray Free-Electron Laser Facility (European XFEL). The European XFEL is currently under construction in the Hamburg region (Figure 1) and is one of the major research infrastructure projects highlighted in the roadmap published by the European Strategy Forum on Research Infrastructures. Founded in 2009 with an intergovernmental agreement, the facility is supported by 11 European countries. From 2017 on, it will provide scientists and industrial researchers with an outstanding new tool to investigate the structure of matter as well as important problems in medical research, new and sustainable energy sources, and the development of materials for new technologies and a better environment.

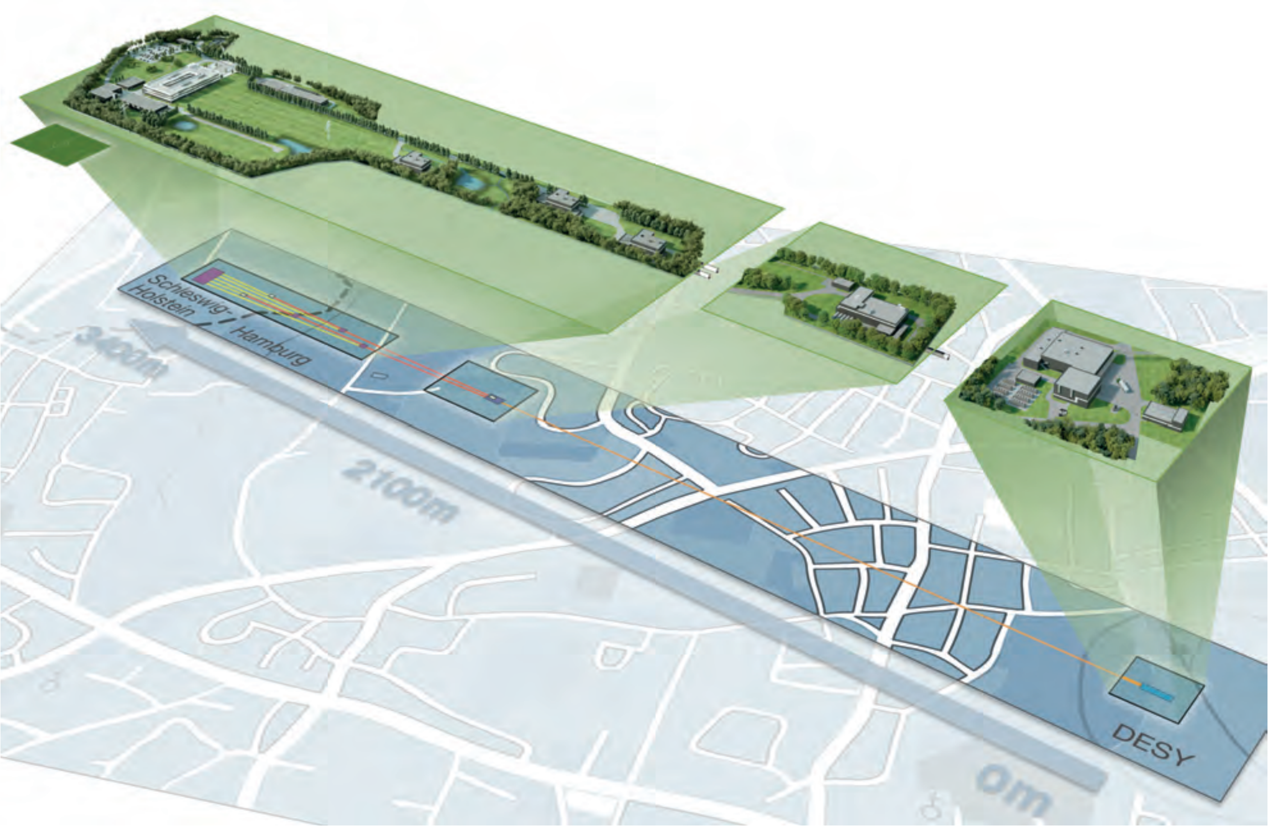


Figure 1: General layout of the European XFEL facility, with the DESY-Bahrenfeld site in Hamburg to the right and the research campus in Schenefeld with the experiment hall on the left. The overall length of the mostly underground facility is approximately 3.4 km, composed of 5.8 km of tunnels.

X-rays are electromagnetic waves, like radio waves, microwaves, or visible light, but with a much shorter wavelength. While no 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 (Figure 2). X-rays range from lower-energy “soft” X-rays, which have wavelengths capable of “seeing” large molecules such as proteins, to higher-energy “hard” X-rays, which have shorter wavelengths that are comparable to individual small molecules and atoms.

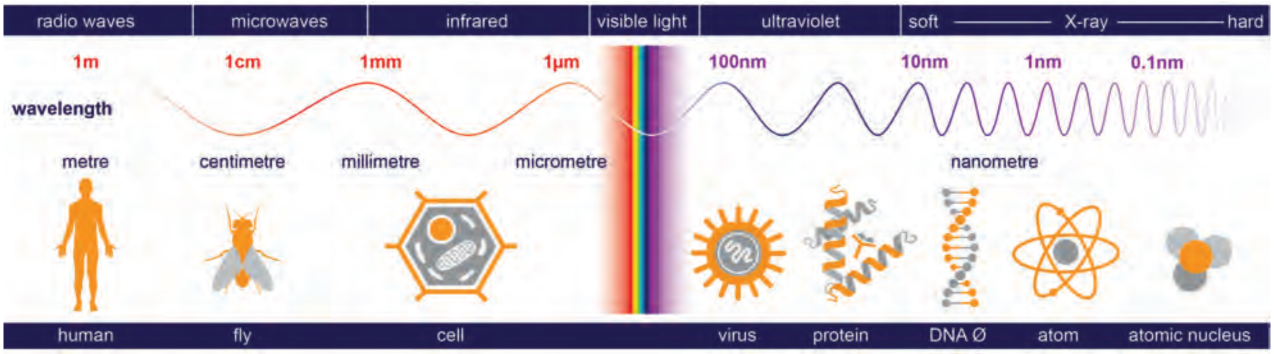


Figure 2: The spectrum of electromagnetic radiation, showing the size of the wavelengths of each type of radiation in comparison to different objects. The shorter the wavelength of the light, the smaller are the objects that can still be “seen” with it.

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—based on X-ray experiments and one of the most important of the century—exemplifies how understanding structure is key to understanding function. This is also very important in other fields, such as chemistry or materials science (see Section 4, “Materials and processes for advanced technologies”).

The determination of complex molecular structures requires very bright X-ray sources. Particle accelerators, in particular electron accelerators, 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 September 2013, this number reached above 94 000; in over 83 000 of these, the structure was determined by synchrotron X-rays. Today, synchrotrons are the most important tool to determine the structure of biomolecules, and six chemistry Nobel Prizes have been awarded for research in which synchrotron sources played a decisive role.

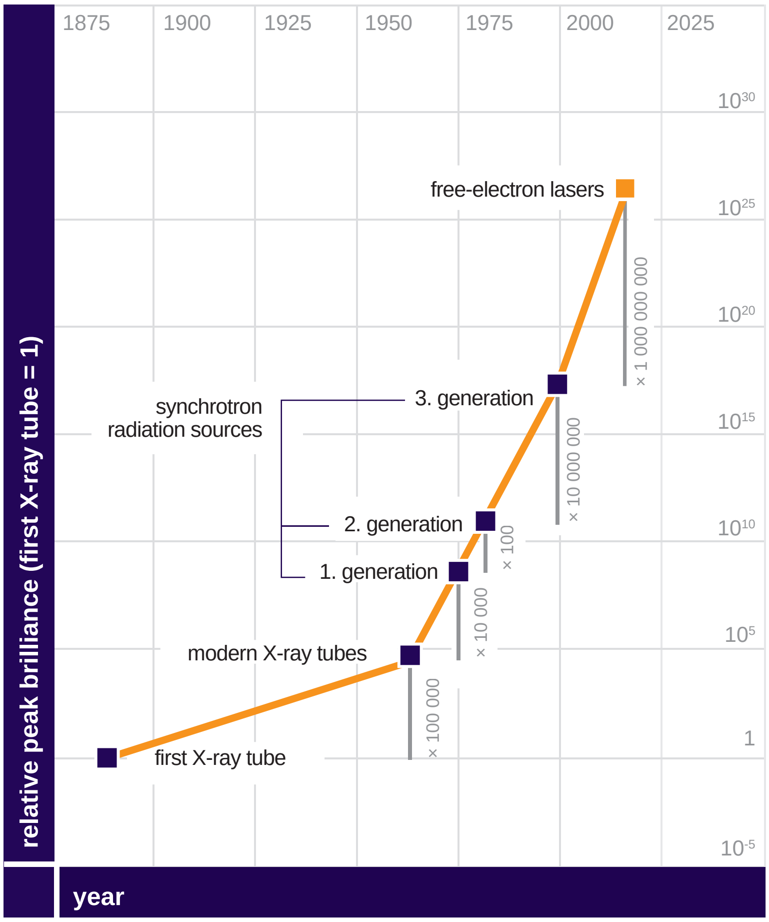


Figure 3: Evolution of peak brilliance.
The development of X-ray radiation sources demonstrates how dramatically the brilliance has increased since the discovery that particle accelerators can produce synchrotron radiation.
The realization of the X-ray free-electron lasers continues this upwards trend and opens up previously undreamt-of possibilities for research.

In the last 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:

1. The FEL pulses are extremely bright, about 100 million to a billion times brighter than the synchrotron X-rays (Figure 3).
2. The FEL pulses are extremely short, down to a few 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 hair.
3. The 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 (Figure 4). This is a quality that makes the X-ray FEL pulses much more useful for experiments than conventional X-rays.

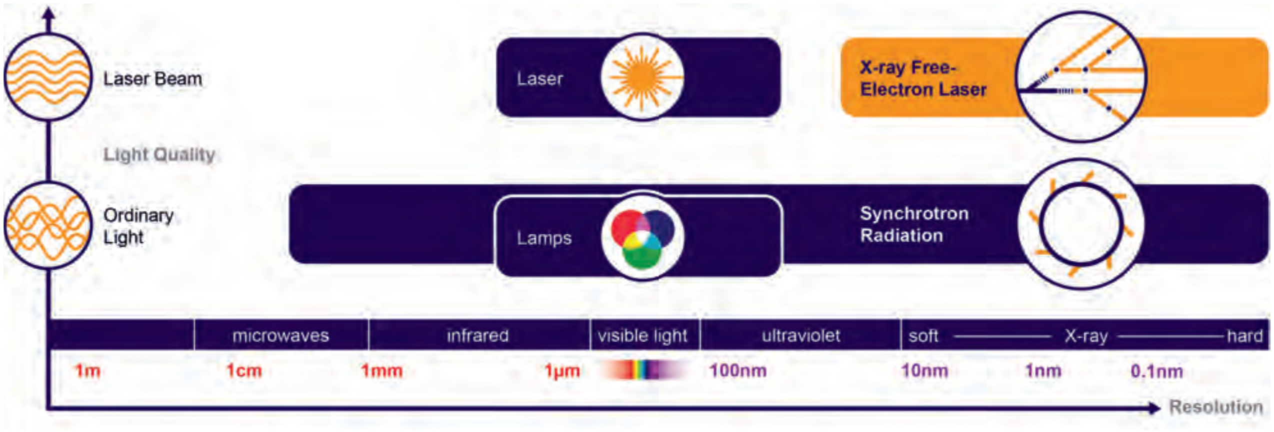


Figure 4: Light quality and wavelengths of different light sources in comparison. Laser beams (which are coherent) have a higher light quality than ordinary light (called incoherent, represented by lamps). Large light source facilities are shown to the right. X-ray free-electron lasers (orange) are capable 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.

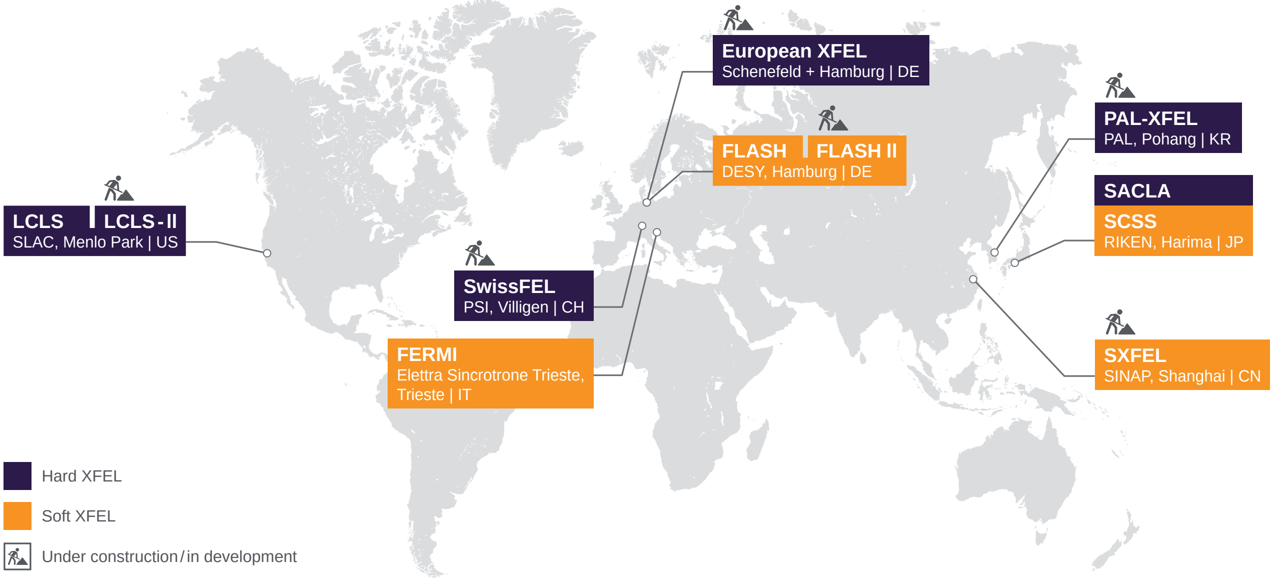


Figure 5: FEL light sources worldwide. Currently, the only hard X-ray FELs accepting users are SACLA in Japan and LCLS in the United States.

Today, there are a handful of X-ray FELs in operation (Figure 5), in Germany (FLASH at DESY in Hamburg), Italy (FERMI@Elettra in Trieste), in the US (LCLS at SLAC in California), and in Japan (SACLA at the RIKEN Harima Institute, Hyogo). LCLS and SACLA are currently the most powerful. Other advanced industrial countries, such as South Korea, are also building X-ray FELs or, like Switzerland, building a national facility in addition to contributing to the construction of the European XFEL.

The European XFEL will be more powerful in terms of electron energy and brightness than the other facilities, and it will produce 27 000 pulses per second, instead of the 60 of SACLA or the 120 of LCLS. This is a very important advance which will put Europe in the lead in this highly competitive scientific and technical environment (Table 1).

Project	**LCLS, USA**	**SACLA, Japan**	**European XFEL**	**SwissFEL, Switzerland**	**PAL XFEL, Korea**
Max. electron energy (GeV)	14.3	8.5	17.5	5.8	10
Wavelength range (nm)	0.13–4.4	0.06–0.3	0.05–4.7	0.1–7	0.06–10
Photons/pulse	~10^{12}	2×10^{11}	~10^{12}	~ 5×10^{11}	10^{11}–10^{13}
Peak brilliance	2×10^{33}	1×10^{33}	5×10^{33}	1×10^{33}	1.3×10^{33}
Pulses/second	120	60	27 000	100	60
Date of first beam	2009	2011	2016	2016	2015

Table 1: Comparison of the properties of hard X-ray light sources, including European XFEL

In the following sections, a few examples demonstrate the importance of X-ray FEL facilities for the progress of science and society.

2 The European XFEL and the health problems of the 21st century

Life expectancy remained essentially unchanged from the earliest times until the middle of the 19th century, when the gradual improvement of hygienic practices and conditions in the developed nations started to have an impact. Progress in modern biomedical sciences, especially since the development of molecular biology in the 20th century, further contributed to an increase of life expectancy worldwide. However, the populations of developing countries are still paying a heavy toll to disease, and, in the developed countries, aging populations have transformed some age-related ailments into widespread social phenomena. In addition, severe epidemics could spread from animal species to humans, as the avian flu or AIDS exemplified. The prevention and cure of disease is based very often on a complete understanding of the causes and the mechanisms of disease development down to the molecular level, and the design of new pharmaceutical products relies on deciphering the atomic details of the structure of biomolecules (Figure 6). This is why researchers from pharmaceutical companies are the most frequent industrial users of synchrotron sources.

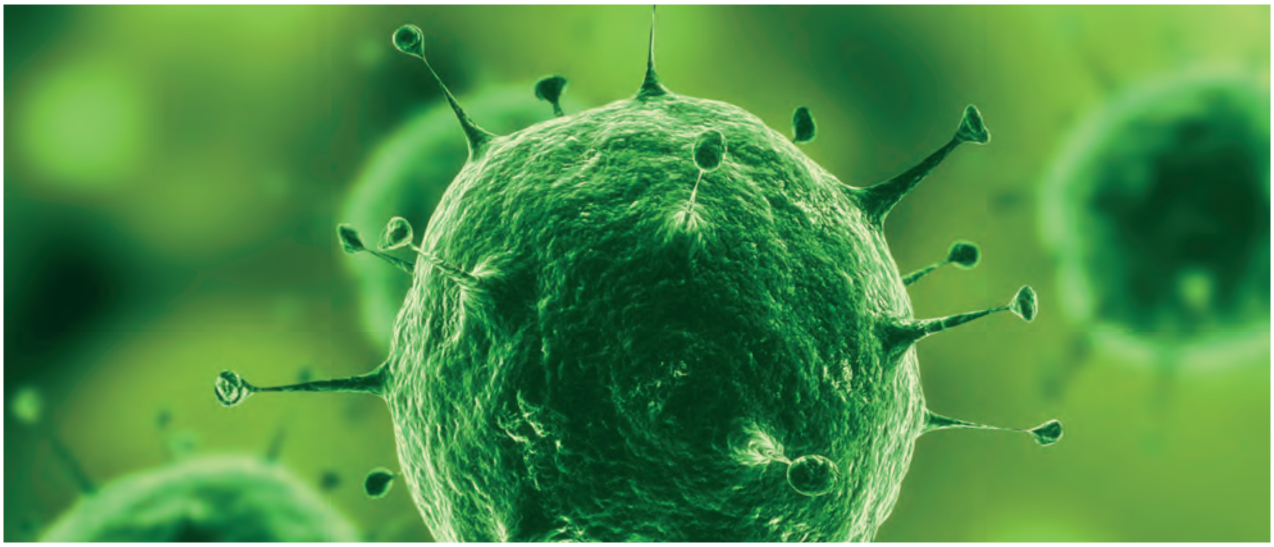


Figure 6: Viruses such as HIV or influenza, with diameters between 80 and 150 nanometres (billionths of a metre) in size, rely on specialized biomechanical and biochemical processes to infect cells. The European XFEL is expected to show in unprecedented detail how these infections occur, possibly unlocking more effective and more targeted treatments for the diseases these viruses cause. Credit: fotolia

The European XFEL's impact on structural investigations will be manifold:

- First of all, thanks to brightness, coherence, and short duration of pulses, researchers will be able to investigate atomic-level structures of biomolecules better and easier than ever before. The short duration of pulses is extremely important because it allows for reduction of the main obstacle to high resolution pictures: the radiation damage by the very action of the intense X-ray pulse. A molecule hit by the beam literally explodes, a process which takes place over many tens or hundreds of femtoseconds (Figure 7). Although this is still just a very short fraction of an instant, it is slow as compared to the duration of the pulses produced at the European XFEL. Therefore, the European XFEL can capture the image encoding the structure before destruction occurs.
- Second, for the same reasons, researchers hope that imaging of biological objects—such as cells, organelles inside cells, and viruses—will be possible with unprecedented resolution of a few nanometres.
- Third, the ultrashort pulses allow dynamic studies of processes—in other words, a transition from a picture to a movie of a molecule in action.

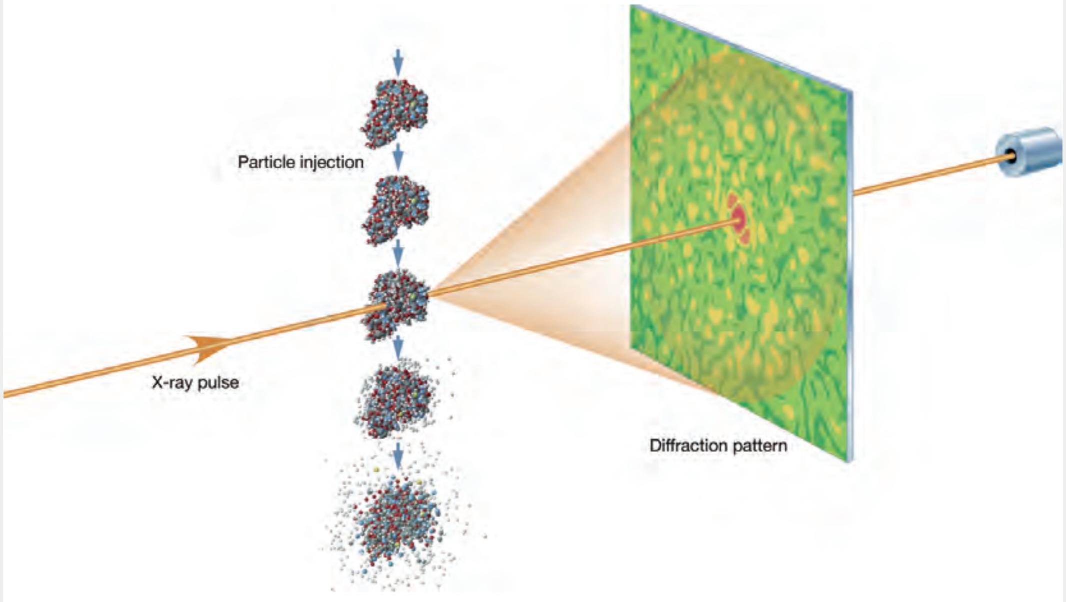


Figure 7: A pulse of X-rays from a free-electron laser illuminates an injected biomolecule. A camera downstream of the interaction region records the diffraction pattern, which contains information about the structure of the molecule before its destruction. Measuring many such diffraction patterns from copies of the same biomolecule will enable scientists to understand its three-dimensional structure.

To determine the arrangement of the atoms in a molecule or material with X-rays, it is currently still necessary to have that molecule or material in a crystalline solid form in which the molecules are placed in the same orientation periodically repeated in space. Crystallization of biological molecules is by no means simple, and the efforts to obtain crystals of sufficient size and quality for synchrotron investigation have lasted years, if not decades, whereas the successive steps are much faster.

X-ray FELs have already shown a qualitative improvement over synchrotrons in the capability to obtain structural information from very small (micrometre or less) nanocrystals. Very recently at LCLS in Stanford, the previously unknown structure of a protein (cysteine protease cathepsin B) was determined, to a resolution of 0.21 nm, from the investigation of nanocrystals at room temperature (Figure 8). The protein plays a very important role in the pathogenesis of sleeping sickness, a disease that is widespread in Africa and causes about 30 000 deaths per year. The researchers hope the new knowledge will lead to a novel treatment approach against the parasite causing the disease.

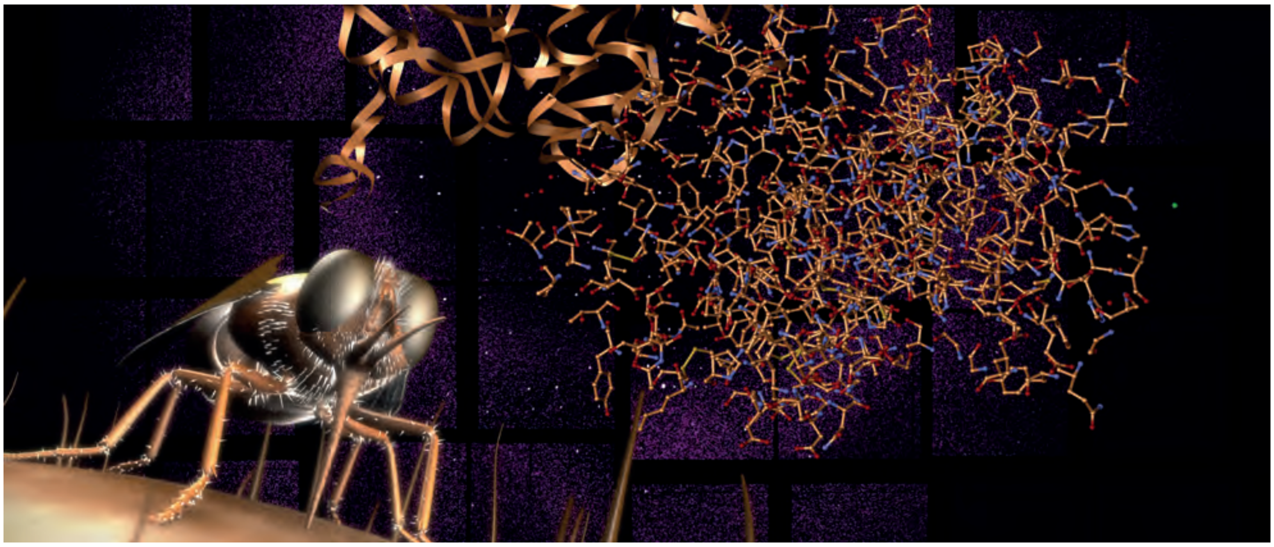


Figure 8: Structure of an important protein involved in the transmission of African sleeping sickness. Scientists created diffraction patterns (shown in background) at LCLS that were then reconstructed into the molecular structure (shown in foreground, not to scale). Credit: Greg Stewart / SLAC National Accelerator Laboratory

The European XFEL pulses are going to improve the already demonstrated structural determination of nanocrystals considerably, and they are expected to pave the way towards the ultimate dream of structural biology, the determination of the structure from single, non-crystallized molecules. The high number of pulses per second will have two major benefits for nanocrystallography: first, the acquisition time will be reduced; and second and even more important, it is estimated that the required quantity of each sample will be about 100 times smaller than that used in the LCLS experiments. In this way, many more experiments can be performed at a small fraction of the cost of the materials, which usually are difficult and expensive to produce and purify. The scientific community expects that the European XFEL will become a very efficient decoder, obtaining in a much shorter time and with reduced effort a large number of structures for molecules such as membrane proteins, from which crystals larger than a micrometre in size are hard to obtain. This will advance progress in our understanding of pathogens and the development of pharmaceutical remedies. But there is another important promise in the future applications of the European XFEL to life sciences: the promise of molecular movies.

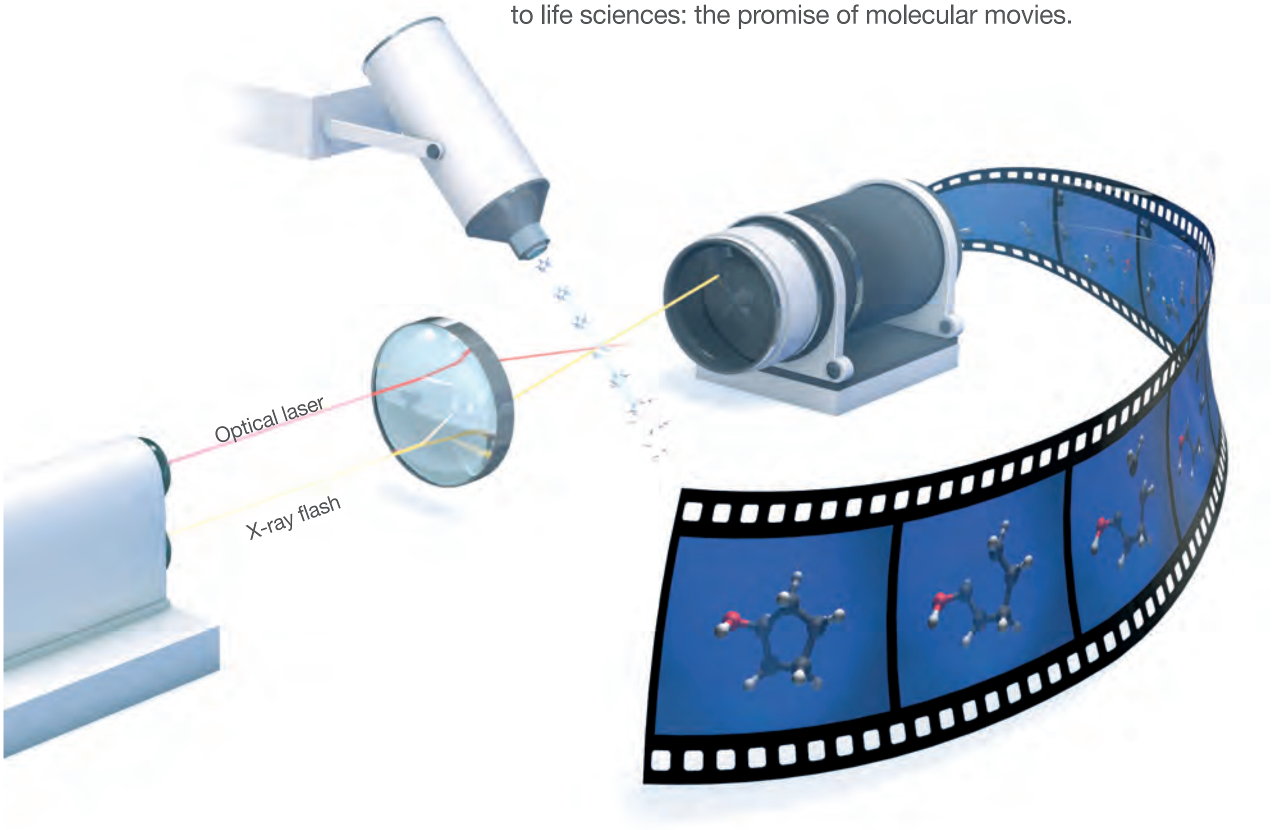


Figure 9: Making molecular movies. First, an optical laser flash triggers a chemical reaction. A second pulse, now from the X-ray FEL, is sent at varying time intervals after the first one to take snapshots of the changes that have occurred in the molecule. Credit: DESY

THE EUROPEAN XFEL AND THE HEALTH PROBLEMS OF THE 21^{ST} CENTURY

Biomolecules are the machines of life. Like mechanical machines with moving parts, they modify their structure in the course of performing their respective tasks. It would be extremely illuminating to follow these modifications and see the motion of the moving parts as in a movie. To make a film of a moving object, it is necessary to take many snapshots. Faster movement requires a shorter exposure time and a greater number of snapshots to avoid blurring the pictures. This is where the ultrashort duration of the FEL pulses will ensure sharp, non-blurred pictures of very fast processes (Figure 9).

A particularly dynamic process in proteins that is not well understood and that plays an important role in the development of many serious diseases is protein folding. In this naturally occurring process, a protein—a linear chain of amino acid molecules—folds into a three-dimensional structure that looks like a tangle and is characteristic of the given protein. In some rare cases, misfolding of a protein occurs, a process which is related to many diseases, such as type-2 diabetes mellitus, Creutzfeldt-Jakob disease, bovine spongiform encephalopathy (mad cow disease), Alzheimer's disease, familial amyloid cardiomyopathy or polyneuropathy, and Huntington’s and Parkinson's diseases. Investigating the folding mechanism and how and why it can go wrong could help in understanding the origin of such very serious illnesses and their prevention. It would therefore be of high interest to explore the very fast elementary steps in this folding process with an X-ray FEL, to map and understand the pathway to protein folding.

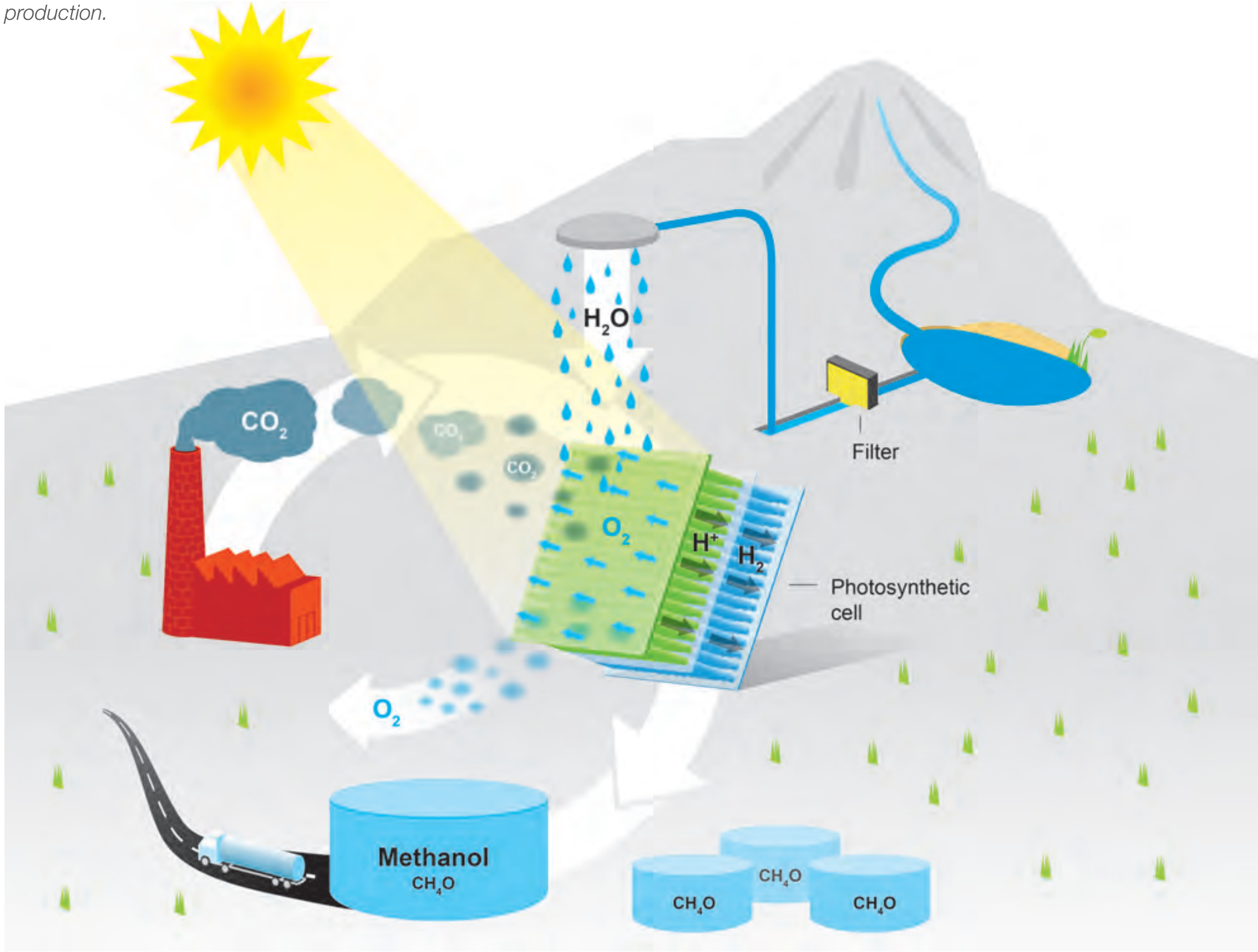
In summary, the European XFEL is expected to enable a giant leap in our ability to investigate, visualize, and understand the molecular basis of biological processes. This includes the development of diseases and the action of natural immune defences such as antibodies; of other biological entities like cells, viruses, or membranes; and of pharmaceutical substances. Research in these areas at the European XFEL will support the long-standing fight for the health of a long-living population.

3 The energy challenge: Natural and artificial photosynthesis

Our society is facing various challenges in providing the necessary energy to support the industrial output and ensure the comfort and transportation requirements of our daily life. Fossil fuels are in limited supply, and their use raises extreme concerns for environment and climate, especially when the rising standard of living and energy requirements of emerging economies are considered. Nuclear fission energy is regarded as a threat by the public, and nuclear fusion is still below the proof-of-principle stage.

The sun delivers enormous amounts of energy to the earth. Clean, economic, and reliable conversion of this abundant energy is a dream for the future. Direct use of solar energy for generating electrical power (photovoltaic devices) or heat (photothermal devices) is confronted with the need to store energy, as the production cycle (up during daytime, down during the night; up on clear days,

Figure 10: Artificial photosynthesis. In the future, biofuels could be produced from CO_2, 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 extreme detail. This will lead to a better understanding of these reactions, enabling scientists to optimize them for highly efficient and clean fuel production.



down on rainy ones; more during summer, less during winter) does not match the consumption cycle. The storage of energy is currently inefficient and expensive, and this limits the photovoltaic and photothermal approach (in analogy to wind power).

In an effort to solve these problems, many scientists are trying to optimize processes which would use sunlight energy to produce storable and transportable fuels, inspired by the natural photosynthetic process in plants, which uses sunlight energy. In plants, the energy of the sun is used to split water into oxygen and hydrogen, the latter of which is further split into a proton and an electron. Their recombination into hydrogen provides the energy to power subsequent reactions that are necessary for the life and growth of plants. Ideally, if one could mimic this process, one could use the hydrogen released from water to react with carbon dioxide and produce methanol or methane, which can be used as fuels (Figure 10).

In nature, the splitting of water molecules and the splitting of hydrogen atoms into protons and electrons takes place in a complex biomolecule, Photosystem II, containing a specific group of four manganese atoms and one calcium atom.

In the laboratory, water can be split with moderate efficiency, but only by employing some rare and heavy metals, such as platinum or ruthenium, that are expensive and very polluting to the environment. It would be a tremendous breakthrough to understand the intermediate steps of the chemistry of water-splitting in plants by such cheap and abundant materials as manganese and calcium, or by similar ones, and to reproduce and optimize the process to improve its efficiency. The full process in plants and bacteria involves the sequential absorption of light from the sun (four photons). Each of the four photons absorbed induces a transformation in the structure of the manganese-calcium complex and one step in the reaction leading to the splitting of two water molecules. The fourth photon brings the complex back to the starting configuration, ready to start all over again.

Studies to elucidate the structures of the manganese calcium complex in the different intermediate states of the process have been hampered so far by the need to freeze the crystals to very low temperatures to limit the effects of radiation damage. Here the FELs have a significant and definite advantage, in the ability for work at room temperature, in which the processes actually take place and can be controlled using successive illuminations with optical laser flashes that drive the complex through the different states of its cycle.

The ability of FELs to follow the steps of such a chemical cycle like in a slow-motion movie could help to better understand the efficient water-splitting reaction in plants. The unique capabilities of the European XFEL could have a major impact on this exciting pursuit and provide the basis for the application of an optimized photosynthetic process on an industrial scale, to generate hydrogen and liquid fuels from ingredients as cheap and abundant as sunlight, water, carbon dioxide, and some light metals.

4 Materials and processes for advanced technologies

4a Catalysis and catalytic reactions

The previous discussion of photosynthesis provides an example of catalysis in chemical reactions: the complex biomolecule containing manganese and calcium is left unchanged by the reaction in which the water molecules are split, but it is not a purely passive spectator. It takes part in some intermediate steps of the process in a way that makes it an indispensable ingredient for an efficient progress of the reaction. The chemists call such a facilitator agent a catalyst, and the process of facilitation catalysis.

Catalysts have been of fundamental importance for the chemical industry for at least 100 years. In the early 20th century, Fritz Haber and Carl Bosch developed catalysts to boost the efficiency of ammonia production from nitrogen and hydrogen, starting the synthetic fertilizer industry. Today, catalysts are also used to limit the environmental damage of car exhaust gases (Figure 11) and are fundamental in the petrochemical industry and in many other applications, with a market of tens of billions of euro.

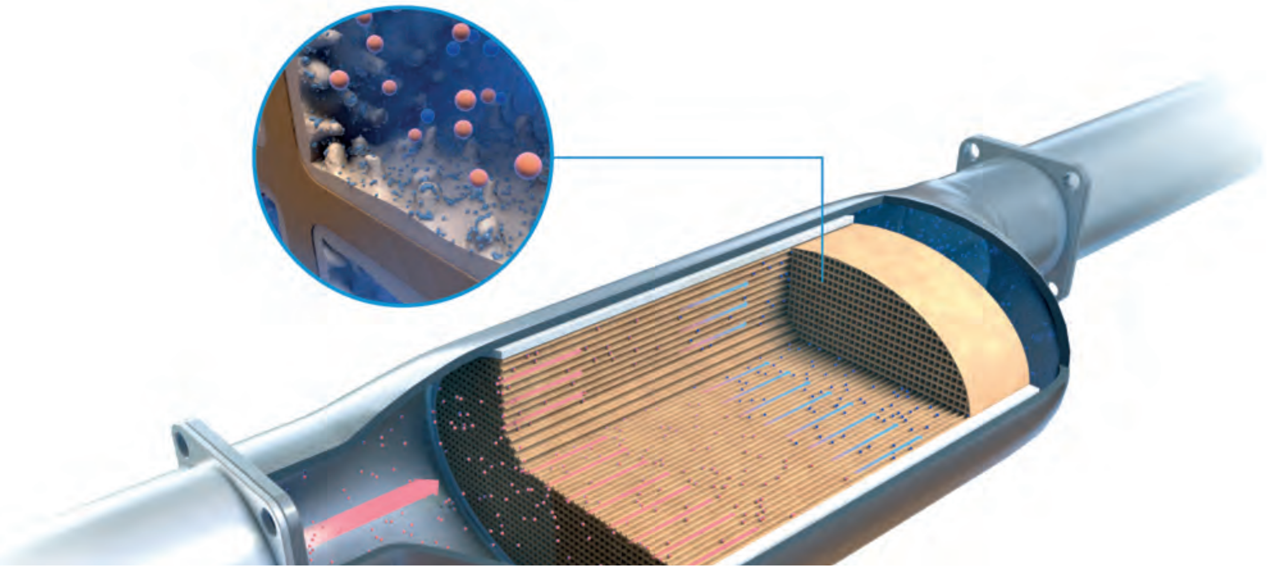


Figure 11: A car's catalytic converter, which helps reduce pollution in the exhaust. The European XFEL could improve the understanding of the process of catalysis and help make more efficient, less toxic catalysts. Credit: DESY

Despite their widespread use, the action of catalysts is very often poorly understood. They have in many cases been developed by trial and error, with what some people call “cooking recipes”. X-ray FELs will give new impulses to systematic approaches based on the possibility to shoot molecular movies of the catalyst’s action in the various stages of a reaction. Understanding the molecular mechanisms in detail will improve the development of better and more environment-friendly catalysts, with important effects on a whole range of important industrial processes.

4b Nano-magnetism and information technology

The development and improvement of materials for the most modern technologies also poses challenges that X-ray FELs can help to solve. Progress in information technology, for example, results from our ability to store information on smaller and smaller areas, and also on the ability to read it and write it as rapidly as possible. Present-day hard disk drives use layered magnetic materials in which the tiny magnetic moment of each grain in the topmost layer can be magnetized in the up or down direction to indicate a “0” or a “1”, thus storing one bit of information. Writing usually takes place by applying magnetic fields; reading occurs by measuring electrical resistance that depends on the orientation of the magnetic moment of the top layer (the so-called “giant magneto-resistance effect”, for which the 2007 Nobel Prize in Physics was awarded to Albert Fert and Peter Grünberg). In recent years it was discovered that a short laser pulse with circularly polarized light, which has two possible directions like a left-turning or right-turning screw, can also write in a sample by changing the magnetic polarity, but more quickly. The European XFEL is going to be equipped with a special device to produce circular polarized X-rays that will permit researchers to obtain a map of the magnetization of a sample and of its evolution in time. This will lead to a better understanding of ultrafast magnetization erasure and re-writing by optical laser pulses and should contribute to establishing the mechanism and approach the physical speed limits of magnetic recording. Faster data recording is a central issue for progress in information technology and for the development of numerous applications and products in science and technology.

5 The European XFEL construction and technology transfer to industry

Even in the construction phase, the European XFEL project has already stimulated the development of some high-technology industrial sectors in the participating countries. To achieve the demanding performance indispensable for the European XFEL, the fabrication of many components requires all the sophisticated know-how of the contributing research labs; on the other hand, these components need to be produced in large series by industry. For example, 800 accelerator resonant cavities, made of a metal called niobium, are needed, plus some pre-series and spare ones. The order was split between two industrial companies that equipped themselves with the necessary infrastructure and were extensively trained through the pre-series production, under the guidance of experts from DESY and from the Italian research agency INFN. The underlying TESLA technology, developed at DESY, is now emerging as a standard for superconducting linear accelerators worldwide, for applications not only in FELs but also in other research infrastructures, such as spallation neutron sources and high-energy physics colliders (Figure 12). The technology is foreseen for various projects in the planning or in the pre-construction phase all over the world, and the companies in question have acquired a solid advantageous position in a market niche that is bound to expand.

Figure 12: The accelerator technology used in the European XFEL, based on these specialized niobium cavities, has already made an impact on the development of linear accelerators worldwide. Credit: DESY

Another area in which the European XFEL has been stimulating a considerable development effort is in detector devices. In order to take complete advantage of the European XFEL's high number of pulses per second, the detector (essentially a digital camera for X-rays) must be able to record a high-quality image on a sensor, transfer it to a temporary memory medium, clear the image from the sensor, and be ready for the next one—all in an extremely short period of time. The temporary memory storage has been designed and prototyped with a capacity for several hundreds of images and with the objective to reach a few thousands in the future. All this requires great sophistication and expertise, so a number of European laboratories were involved in the development of prototypes. Advanced electronic integrated circuits were designed and their fabrication was given out to companies. Some features of the imaging detectors with very high read-out speed will be of interest not only for future high repetition rate FELs but also for research with synchrotrons, and possibly in other areas, including commercial electronic devices, where speed of data processing and of data storage and recovery could open up new business opportunities.

All the information acquired during an experiment (hundreds of thousands and sometimes millions of images) must be transferred to memory. In addition, all images must be accompanied by additional information (metadata) allowing identification of the image (for example, to which experiment and sample it belongs and the settings of the different pieces of apparatus). In this way, the European XFEL contributes to the general area of current research and development that goes under the name “data deluge”, which increasingly affects not only the scientific enterprise in general (one example: the experiments at CERN that led to the celebrated discovery of the Higgs Boson) but also many aspects of business and public services in our digital age. Richard Feynman estimated in 1959 that the total information contained at the time in the major libraries of the world (24 million books) amounted to 0.1 petabytes of information (or 1014 bytes). In more modern terms, this amount of information can be stored in about 10 000 high-quality DVDs; nonetheless, the European XFEL is expected to produce an equivalent amount of information within the first few months of experiment time—and this rate will only increase! Some of the solutions being developed for dealing efficiently with the data deluge at the European XFEL and other large research infrastructures like CERN are expected to be of use in other parts of society as well: better weather forecasting, more accurate climate evolution simulations, and global communication networks, where the amount of data is growing inexorably, albeit at a slower pace.

6 Concluding remarks

The European XFEL—a large and 3.4 km long research facility in the Hamburg region constructed by 11 European countries and mostly located in underground tunnels and halls—will be a major contribution to consolidating Europe's position at the forefront of basic scientific research. It holds the promise of many exciting discoveries for the benefit of society, a few examples of which we have presented in the preceding paragraphs.

The very construction of the facility poses scientific and technological challenges that are being addressed with the help of academia and industry, to the advantage of both.

In operation, the European XFEL will select the best and most innovative experiments proposed by researchers from many different disciplines, providing an opportunity to access a unique instrument. Thus, this opportunity will also be available to young scientists at the beginning of their careers, to those working in institutes or universities with modest funding, as long as their ideas are bright and show promise to lead to a real advance in a field of science. With 6 instruments in the starting configuration and the possibility to upgrade to up to 15, the European XFEL will be able to host more researchers than any other X-ray FEL in the world. Located within a cluster of prestigious institutions—such as DESY, CFEL, the University of Hamburg and the Max Planck Institutes, EMBL, CSSB, and others—the European XFEL will maximize synergies and collaborations to offer a unique and stimulating research environment.
The conclusion of the construction project in a few years will place Europe at the top of the league of X-ray sources. It is expected that the European XFEL will be yet another success story of the European collaboration in science and technology.

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