# femto

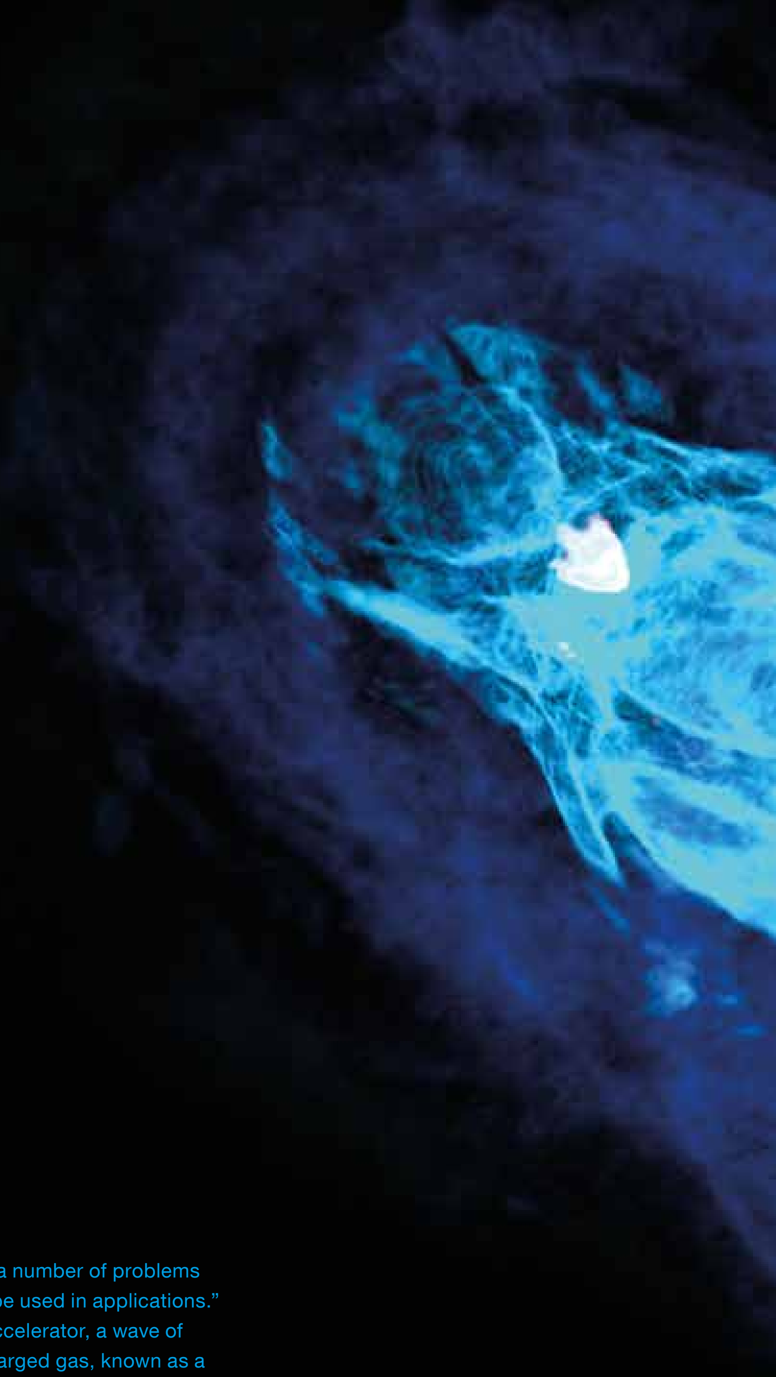
The DESY research magazine – Issue 02/17


**Mixed doubles**
Analysis reveals two different forms of water

**Extreme ionisation**
X-ray flash creates "molecular black hole"

**Superhard windows**
Silicon ceramic becomes transparent at high pressure

DESY

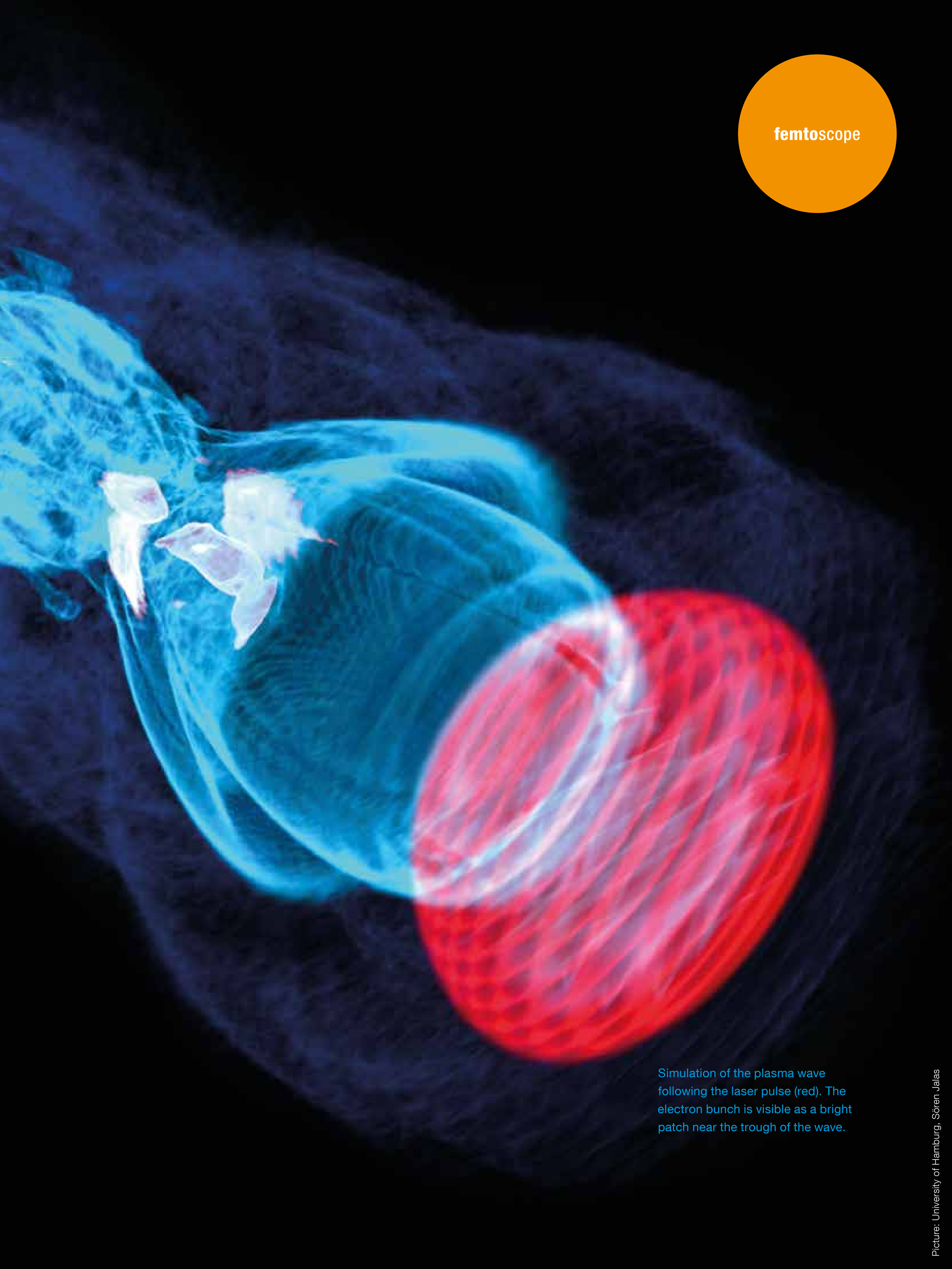


## Pendulum trick for plasma accelerators

Scientists in Hamburg have come up with an ingenious way of improving so-called plasma accelerators, which are considered promising candidates to become the particle accelerators of the future. The quality of the electron beams produced by these innovative particle accelerators can be substantially improved by adding an oscillating component. “Plasma accelerators can achieve up to a thousand times higher accelerations than the most cutting-edge machines in use today,” says Reinhard Brinkmann, the director of DESY’s Accelerator Division, on whose proposal the study was based. “This would make it possible to build more compact and more powerful devices for a wide range of applications, from fundamental research through to medicine. However, the technology is still in its very early experimental stages, and we will have to solve a number of problems before it can be used in applications.”

In a plasma accelerator, a wave of electrically charged gas, known as a plasma, is produced inside a thin capillary. This gas could be hydrogen, for example, subjected to extremely intense and short laser pulses. As the researchers have calculated, the acceleration of electrons by the plasma wave is considerably more uniform when the electron bunches swing to and fro across the wave. “We are hoping that the principle we have come up with will give us direct control over the accelerating field. This would be a crucial step towards the development of plasma accelerators,” says main author Andreas R. Maier from the University of Hamburg.

*Physical Review Letters, 2017; DOI: 10.1103/PhysRevLett.118.214801*



Simulation of the plasma wave following the laser pulse (red). The electron bunch is visible as a bright patch near the trough of the wave.

Picture: University of Hamburg, Sören Jalas

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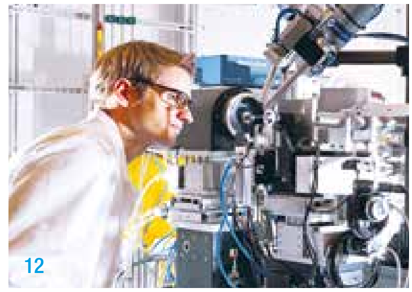
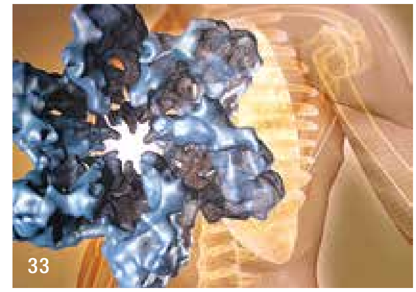
### How does innovation arise?

Whenever research and development take place, innovation – the emergence of something new – is never far behind. This might be an overarching model of how the universe arose, or a ground-breaking technology that makes it possible to observe single atoms. In the narrow sense, an innovation can first be said to have crystallised out of a wealth of new ideas and discoveries when it becomes commercially exploitable. A research centre like DESY generates both fundamental knowledge leading to the innovations of the future, and industry-oriented applications and spin-offs. Ideally, these two aspects mesh perfectly, helping to ensure our society is up to the challenges of the future.







## CAMPUS



## ZOOM



## SPECTRUM



## SECTIONS

# Water is not just water


Liquid water has two variants: high-density liquid (HDL) and low-density liquid (LDL), which have now been observed at extremely low temperatures – but can not be bottled.

Picture: DESY, Gesine Born

Liquid water exists in two different forms – at least at very low temperatures. This is the conclusion drawn from X-ray experiments carried out at DESY and at the Argonne National Laboratory in the USA by an international team of researchers headed by the University of Stockholm. The scientists led by Anders Nilsson had been studying so-called amorphous ice. This glass-like form of frozen water has been known for decades. It is quite rare on Earth and does not occur in everyday life; however, most water ice in the solar system actually exists in this amorphous form. Instead of forming a solid crystal – as in an ice cube taken from the freezer – the ice takes on the form of disordered chains of molecules, more akin to the internal structure of glass. Amorphous ice can be produced, for example, by cooling liquid water so rapidly that the molecules do not have enough time to form a crystal lattice.

"Amorphous ice exists in two varieties: one with a high and one with a low density," explains Felix Lehmkühler, a physicist from DESY who was a member of the research team. These two varieties are referred to as high-density amorphous (HDA) ice and low-density amorphous (LDA) ice. "HDA ice is some 25 percent denser than LDA ice," Lehmkühler adds. "Scientists have been wondering for some time whether these two varieties of ice might be associated with corresponding varieties of liquid water. However, that is very difficult to measure. Even if water does exist in two states, they will constantly be mixing with and turning into each other, and there is no way of separating the two." The scientists have now managed to overcome this obstacle at low temperatures. In the Stockholm laboratory, Katrin Amann-Winkel prepared extremely pure samples of HDA ice. At the Argonne National Laboratory, the scientists noticed that the internal structure of this ice changed upon warming between temperatures of minus 150 to minus 140 degrees Celsius – turning into a lower-density form.

> *"The new remarkable property is that we find that water can exist as two different liquids at low temperatures"*
>
> *Anders Nilsson, University of Stockholm*

The scientists then observed the dynamics of this phase change at DESY's X-ray source PETRA III. They found that the transition takes place via a liquid state: first, the HDA ice turns into a liquid form of high density, then this high-density liquid (HDL) turns into a lower-density form (low-density liquid, LDL). This demonstrates the existence of the two suspected varieties of liquid water – at least at very low temperatures. The extremely low-temperature water is so viscous that the two liquid phases are only transformed into each other and only mix very slowly, allowing this process to be measured.

"The new remarkable property is that we find that water can exist as two different liquids at low temperatures where ice crystallisation is slow," says Nilsson, a professor of chemical physics at the University of Stockholm. "It is very exciting to be able to use X-rays to determine the relative positions of the molecules at different times," adds Fivos Perakis of the University of Stockholm, who was one of the two principal authors of the study, along with Amann-Winkel. "We have in particular been able to follow the transformation of the sample between the two phases at low temperatures and to demonstrate that there is diffusion as is typical for liquids."

The discovery of the two varieties of water does not have any particular consequences for our everyday lives. For scientists, though, it is an important step towards understanding this extraordinary liquid. "Water may seem very simple, but it behaves very strangely compared with other liquids," explains Lehmkühler, a member of the DESY research group for Coherent X-ray Scattering, headed by DESY leading scientist Gerhard Grübel.

> *"Many of these properties are the foundation for the existence of life, because without water and its special properties, life as we know it could not exist."*
>
> *Felix Lehmkühler, DESY*

"Water displays so many anomalies – its density, heat capacity and thermal conductivity to name just three of several dozen properties that distinguish water from most other liquids," notes Lehmkühler. "Many of these properties are the foundation for the existence of life, because without water and its special properties, life as we know it could not exist." This is just one reason why the study of water is so important and a field in which DESY is increasingly involved. New X-ray sources, such as the recently inaugurated European XFEL X-ray laser, whose principal shareholder DESY is, and PETRA IV, the upgraded next generation of DESY's synchrotron source PETRA III, will allow scientists to penetrate even further into the uncharted territory of water's phase diagram.

The scientists are hoping that future experiments will help them to answer questions such as whether the two types of liquid water also exist at room temperature. In principle, there is no reason why they should only occur at low temperatures. "The new results give very strong support to a picture where water at room temperature can't decide in which of the two forms it should be, high or low density, which results in local fluctuations between the two," says Lars Pettersson, professor of theoretical chemical physics at the University of Stockholm. "In a nutshell: Water is not a complicated liquid, but two simple liquids with a complicated relationship."

*Proceedings of the National Academy of Sciences, 2017; DOI: 10.1073/pnas.1705303114*

When HDA ice changes to LDA ice upon warming, it suddenly grows in volume by about a quarter, as had been observed before.

Pictures: University of Stockholm, Katrin Amann-Winkel/Filippo Cavalca

# A molecular black hole

Scientists have used an ultrabright pulse of X-ray light to turn an atom in a molecule briefly into a sort of electromagnetic "black hole". Unlike a black hole in space, the X-rayed atom does not draw in matter from its surroundings through the force of gravity, but electrons with its electrical charge – causing the molecule to explode within the tiniest fraction of a second. The study provides important information for analysing biomolecules using X-ray lasers.

The researchers used the LCLS X-ray laser at the SLAC National Accelerator Laboratory in the USA to bathe iodomethane ($CH_3I$) molecules in intense X-ray light. The pulses reached intensities of 100 quadrillion kilowatts per square centimetre. The high-energy X-rays knocked 54 of the 62 electrons out of the molecule, creating a molecule carrying a positive charge 54 times the elementary charge. "As far as we are aware, this is the highest level of ionisation that has ever been achieved using light," explains Robin Santra from the research team, who is a leading DESY scientist at the Center for Free-Electron Laser Science (CFEL) in Hamburg.

This ionisation does not take place all at once, however. "The methyl group $CH_3$ is in a sense blind to X-rays," says Santra, who is also a professor of physics at the University of Hamburg. "The X-ray pulse initially strips the iodine atom of five or six of its electrons. The resulting strong positive charge means that the iodine atom then sucks electrons away from the methyl group, like a sort of atomic black hole." In fact, the force exerted on the electrons is considerably larger than that occurring around a typical astrophysical black hole of ten solar masses. "The gravitational field due to a real black hole of this type would be unable to exert a similarly large force on an electron, no matter how close you brought the electron to the black hole," explains Santra.

The process happens so quickly that the electrons that are sucked in are then catapulted away by the same X-ray pulse. The result is a

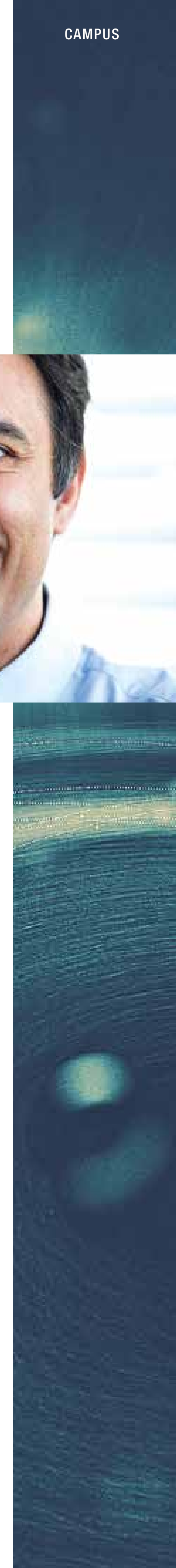
*"As far as we are aware, this is the highest ionisation ever achieved using light"*
Robin Santra, DESY/CFEL

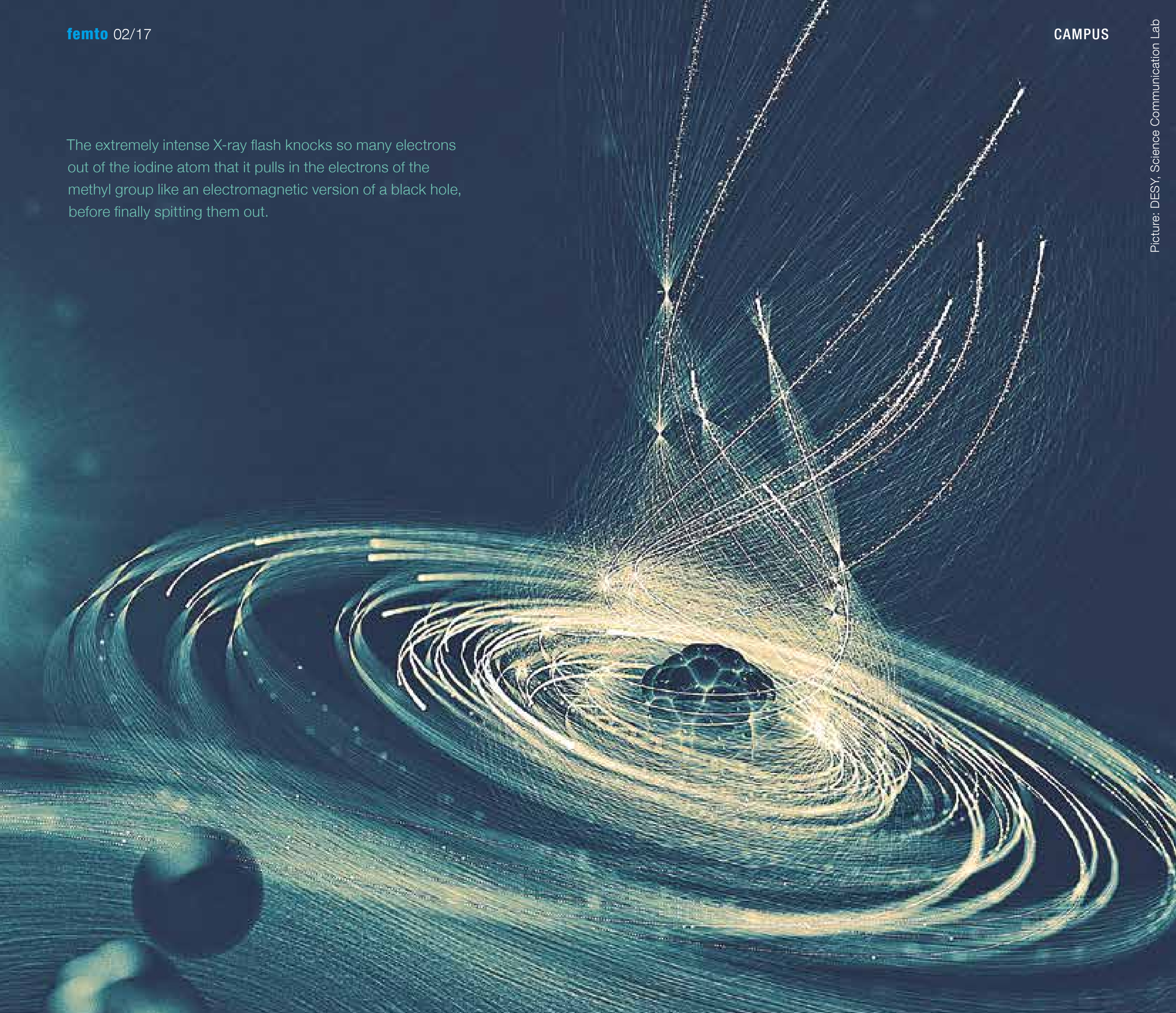
chain reaction in the course of which up to 54 of iodomethane's 62 electrons are torn away – all within less than a trillionth of a second. "This leads to an extremely high positive charge building up within the space of a ten-billionth of a metre. That rips the molecule apart," says Daniel Rolles from DESY and Kansas State University in the USA.

Observing this ultrafast dynamic process is highly significant to the analysis of complex

*"The data are highly relevant to studies using X-ray free-electron lasers, because they show in detail what happens when radiation damage is produced."*
Sang-Kil Son, CFEL

molecules using X-ray free-electron lasers (XFELs) such as LCLS in California and the European XFEL in the Hamburg region. These facilities produce extremely high-intensity X-rays, which can be used, among other things, to determine the spatial structure of complex molecules down to the level of individual atoms. Biologists, for example, can use this structural information to determine the precise mechanism by which





The extremely intense X-ray flash knocks so many electrons out of the iodine atom that it pulls in the electrons of the methyl group like an electromagnetic version of a black hole, before finally spitting them out.

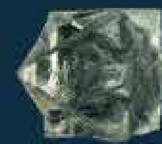
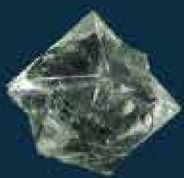
Picture: DESY, Science Communication Lab

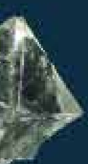
biomolecules work. The molecules reveal their atomic structure before exploding, as other scientists have already shown. However, to study the dynamics of biomolecules, during photosynthesis for example, it is important to understand how X-rays affect the electrons.

In this study, iodomethane served as a model system. "Iodomethane is a comparatively simple molecule for understanding the processes taking place when organic compounds are damaged by radiation," says Artem Rudenko from Kansas State University. "If more neighbours than a single methyl group are present, even more electrons can be sucked in."

Santra's group at CFEL has for the first time managed to describe these ultrahigh-speed dynamics in theoretical terms too. This was made possible by the development of a new computer program, the first of its kind in the world. "This is not only the first time that this experiment has been successfully carried out; we even have a numerical description of the process," points out Sang-Kil Son from CFEL, who was in charge of the team that developed the computer program. "The data are highly relevant to studies using X-ray free-electron lasers, because they show in detail what happens when radiation damage is produced."

*Nature, 2017; DOI: 10.1038/nature22373*



Cristobalite crystals from Harvard Mineralogical Museum, found at Ellora caves in India

# Meteorite mystery solved

Using intense X-ray light produced by particle accelerators, a research team around Leonid Dubrovinsky from the University of Bayreuth in Germany has found the long-sought explanation for apparently contradictory properties of meteorites from Mars and the moon. The team has found out why different forms of silica can coexist in meteorites, although they form under vastly different conditions.

The scientists investigated a silicon dioxide ($SiO_2$) mineral called cristobalite. “This mineral is of particular interest when studying planetary samples such as meteorites, because this is the predominant form of silica in extraterrestrial materials,” explains Ana Ĉernok from the Bavarian Research Institute of Experimental Geochemistry and Geophysics (BGI) at the University of Bayreuth, who is now based at the Open University in the UK. “Cristobalite has the same chemical composition as quartz, but its structure is significantly different,” adds Razvan Caracas from the French research centre CNRS.

In contrast to quartz, which is ubiquitous on Earth, cristobalite is relatively rare on our planet, as it only forms at very high temperatures under special conditions. But it is quite common in meteorites that were ejected from the moon or from Mars by asteroid impacts and finally fell to Earth.

Surprisingly, researchers have also found the mineral seifertite together with cristobalite in Martian and lunar meteorites. Seifertite is another version of silica, but needs extremely high pressures to form. It was first synthesised by Dubrovinsky and his colleagues 20 years ago. “Finding cristobalite and seifertite in the same grains of meteorite material is enigmatic, as they form under vastly different pressures and temperatures,” underlines Dubrovinsky. “Triggered by this curious observation, the behaviour of cristobalite at high pressures has been examined in numerous experimental and theoretical studies for more than two decades, but the puzzle could not be solved.”

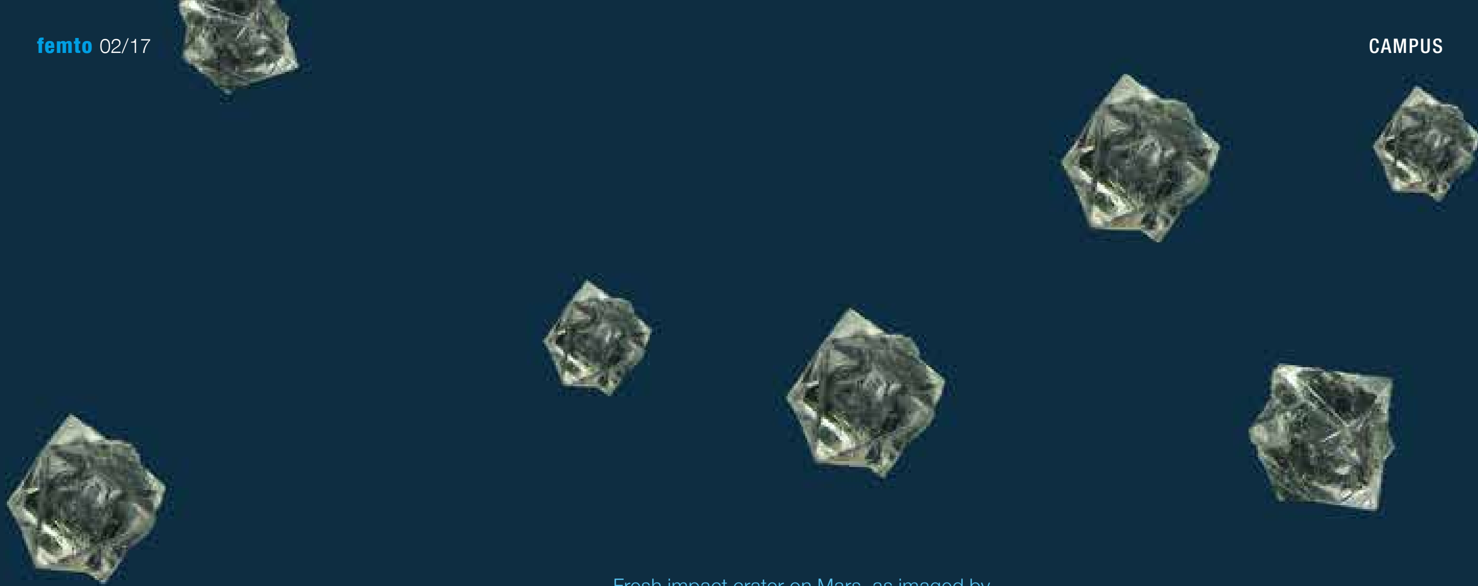
Using the intense X-rays from the research light sources PETRA III at DESY and ESRF in Grenoble, France, the scientists could now get unprecedented insights into the structure of cristobalite under high pressures of up to 83 gigapascals (GPa), which corresponds to roughly 820 000 times the atmospheric pressure. “The experiments showed that when cristobalite is compressed uniformly or almost uniformly – or as we say, under hydrostatic or quasi-hydrostatic conditions – it assumes a high-pressure phase labelled cristobalite X-I,” explains Elena Bykova, who works at the PETRA III beamline where the experiments took place. “This high-pressure phase reverts back to normal cristobalite when the pressure is released.”

*“These results have immediate implications for studying impact processes in the solar system”*

*Leonid Dubrovinsky, University of Bayreuth*

But if cristobalite is compressed unevenly under what scientists call non-hydrostatic conditions, it unexpectedly converts into a seifertite-like structure, as the experiments have now shown. This structure forms under significantly less pressure than is necessary to form seifertite from ordinary silica. “The *ab initio* calculations confirm the dynamical

Pictures: RRUFF Project/University of Arizona



stability of the new phase up to high pressures," says Caracas.

Moreover, it also remains stable when the pressure is released. "This came as a surprise," says Ĉernok. "Our study clarifies how squeezed cristobalite can transform into seifertite at much lower pressure than expected. Therefore, meteorites that contain seifertite associated with cristobalite have not necessarily experienced massive impacts." The unexpected behaviour explains why cristobalite and seifertite can coexist in a meteorite. During an impact, the propagation of the shock wave through the rock can create very complex stress patterns with intersecting areas of hydrostatically and non-hydrostatically compressed materials, so that different versions of silica can form in the same meteorite.

"These results have immediate implications for studying impact processes in the solar system," underlines Dubrovinsky. "They provide clear evidence that neither cristobalite nor seifertite should be considered as reliable tracers of the peak shock conditions experienced by meteorites." But the observations also show more generally that the same material can react very differently to hydrostatic and non-hydrostatic compression, as Dubrovinsky explains: "For materials sciences, our results suggest an additional mechanism for manipulating the properties of materials. Apart from pressure and temperature, different forms of mechanical stress may lead to completely different behaviour of solid matter."

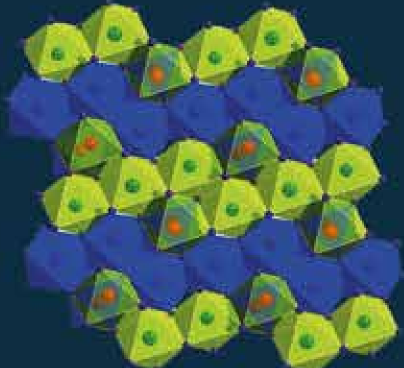
*Nature Communications, 2017; DOI: 10.1038/ncomms15647*

Fresh impact crater on Mars, as imaged by the HiRISE camera on board NASA's Mars Reconnaissance Orbiter

Picture: NASA/JPL/University of Arizona

Leonid Dubrovinsky

Picture: Univ. Bayreuth



Picture: Leonid Dubrovinsky, University of Bayreuth

Model of the crystal structure of cristobalite X-I. This high-pressure phase of cristobalite is composed of two layers (green and blue), each of which consists of $Si_6O$.

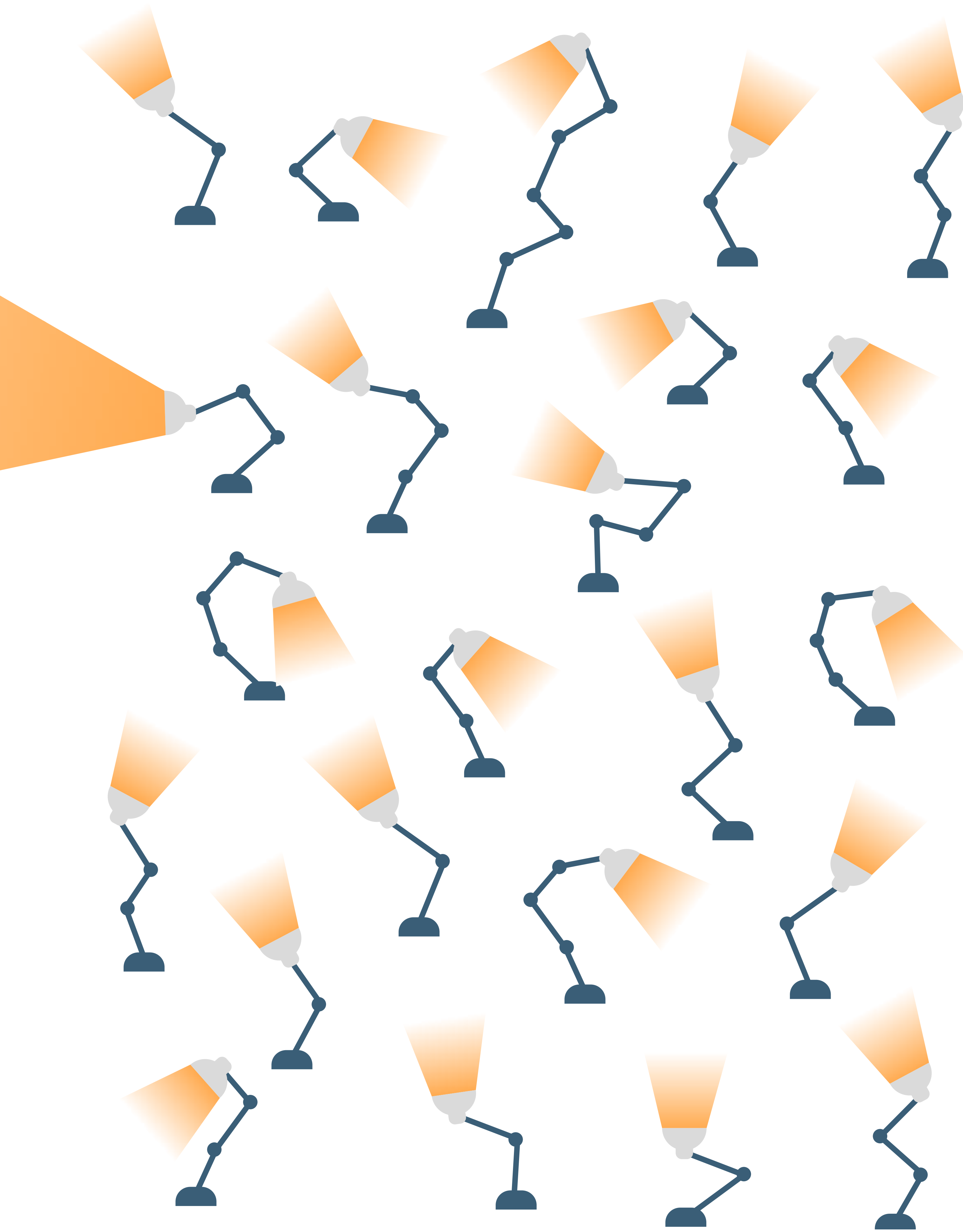
ZOOM

# THINK ANEW!

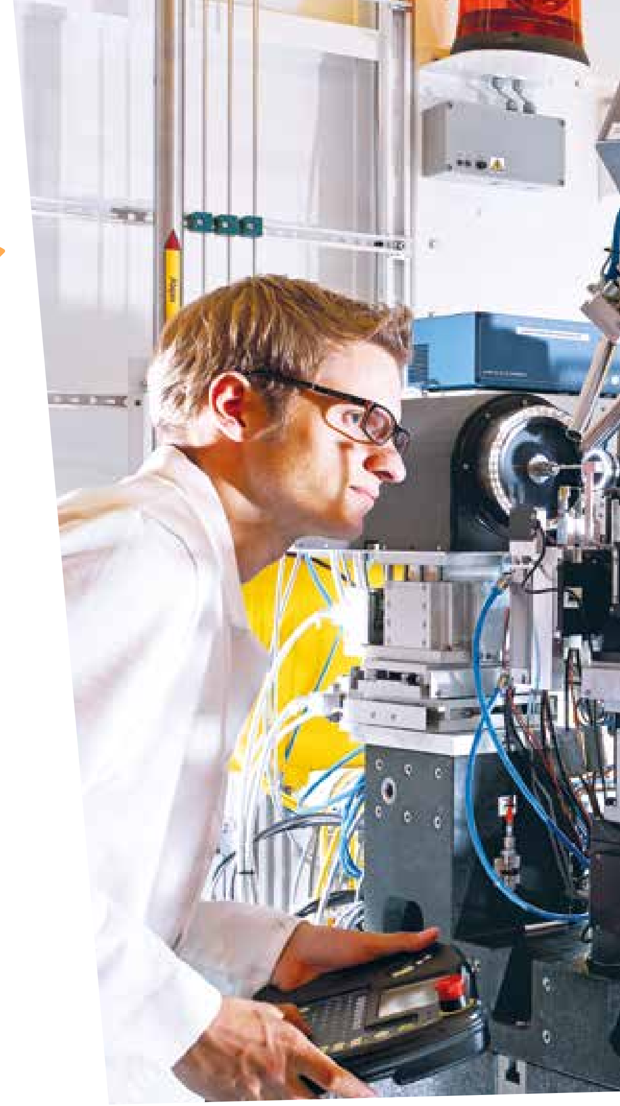
## How does innovation arise?

Whenever research and development take place, innovation – the emergence of something new – is never far behind. This might be an overarching model of how the universe arose, or a groundbreaking technology that makes it possible to observe single atoms. In the narrow sense, an innovation can first be said to have crystallised out of a wealth of new ideas and discoveries when it becomes commercially exploitable. A research centre like DESY generates both fundamental knowledge leading to the innovations of the future, and industry-oriented applications and spin-offs.

Ideally, these two aspects mesh perfectly, helping to ensure our society is up to the challenges of the future. The radical changes sparked by the digital revolution have shortened innovation cycles in industry. As a result, competition has intensified and the pace of social change has accelerated. Science too must take on these challenges. With its broad-based research campus, DESY has the extensive expertise required to drive innovation.



At the P11 experimental station of DESY's X-ray radiation source PETRA III, biomolecules are analysed with atomic precision.



Innovation is one of those buzzwords that energises businesses and politicians alike. Innovations spring from the fertile ground of bright ideas that are transformed into new products, services and processes. "Think anew" is therefore the motto for our times – and for a growing number of companies. A whole philosophy – along with a burgeoning training and service industry – is now dedicated to analysing and explaining how this best works. Innovation consultants and "future shapers" strive to broaden our all-too-narrow horizons with approaches that are unconventional, creative and solution-oriented. Design thinking is the name of a method now being adopted at major companies such as Deutsche Telekom, IBM, Bosch and Daimler. What unites these big names is less a simple desire for the new than a need to stay flexible and innovative in the face of the digital revolution and other challenges, and thereby remain competitive.

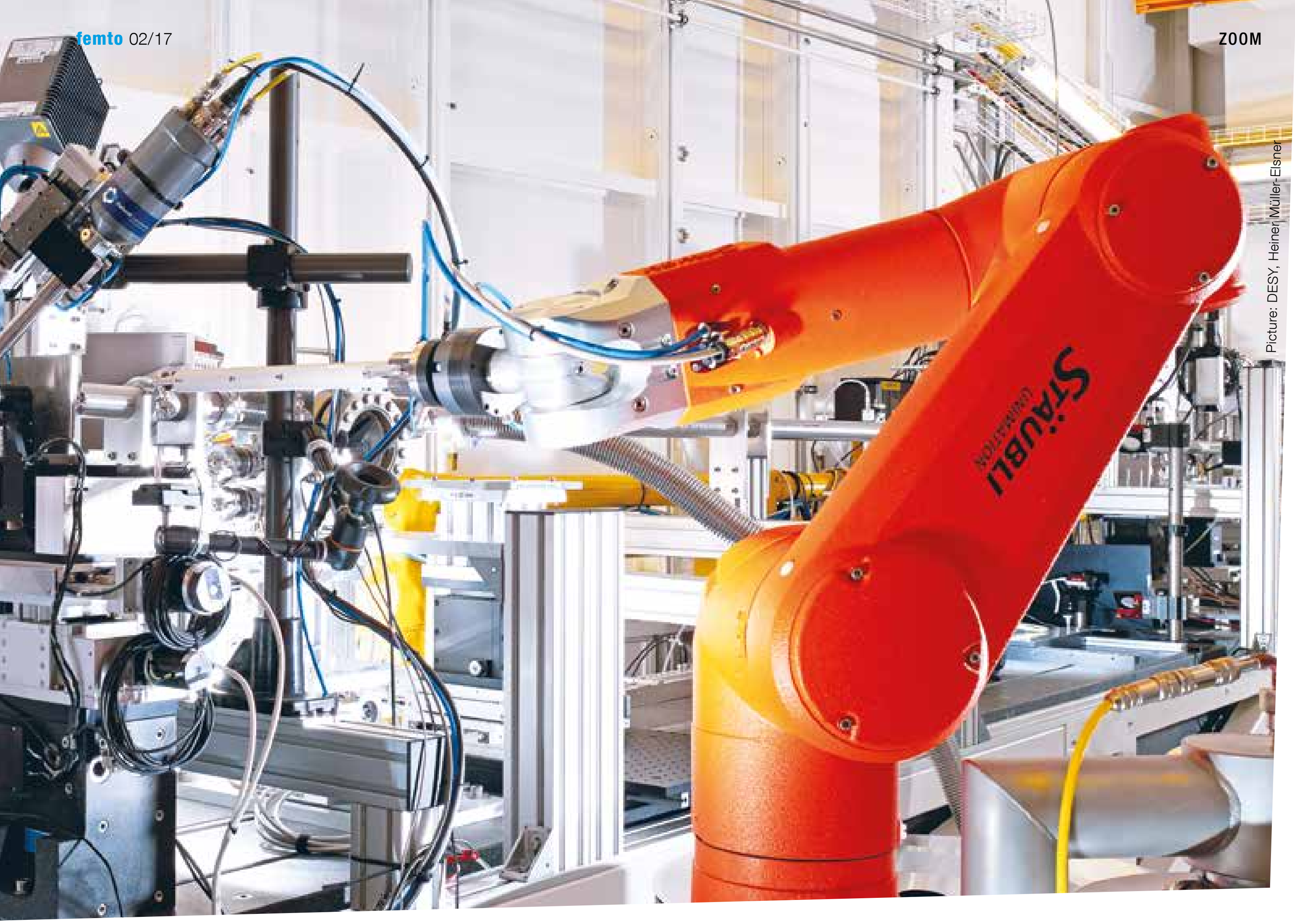
"We have excellent scientists here and an abundance of innovations that arise more or less as a by-product of the work in R&D"

**HELMUT DOSCH**
*DESY*

The new method is easily described: Design thinking is based on the approach used by industrial designers, whereby the key focus is on the users and their needs. The aim is to generate new ideas and develop solutions capable of convincing the people who use them. That might sound logical, but it is by no means a given at companies featuring rigid hierarchical structures and top-down strategies. By contrast, design thinking encourages a networked approach within a team of different specialisations, where people work together in a creative climate, puzzle away at a problem, develop new concepts tailored to the needs of real users, try out new approaches and develop prototypes. Having started life as a simple innovation technique, design thinking has since become a stand-alone method of thinking and working that is not only taught as a subject at Stanford University in California but has also been adopted by a growing number of German companies. Viewed in this way, innovation is by no means something merely to be found in R&D departments. Ideally, it should permeate the entire organisation, informing both strategy and processes as well as the corporate culture.

## SCIENCE AS A DRIVER OF INNOVATION

The approaches that some well-established companies have to relearn using design thinking or other innovation strategies is something that the scientific community, however, employs as a matter of course: rethinking assumptions, constructing hypotheses, questioning accepted wisdom and finding correlations. In other words, science has plenty to offer in terms of innovation. Its whole way of thinking and acting is geared towards discovering new knowledge and methods. "Whenever we do research and devise experiments for that research, innovation just happens naturally," says the physicist Arik




Picture: DESY, Heiner Müller-Elsner

Willner, Chief Technology Officer (CTO) at DESY. That's why science is an ever greater source of new momentum and driver of innovation in society. "We're radically reorganising the way we promote innovation on campus," explains Helmut Dosch, Chairman of the DESY Board of Directors. "We have excellent scientists here and an abundance of innovations that arise more or less as a by-product of the work in R&D. These new developments can make a great contribution to the innovation strategy of the City of Hamburg as well as that of the European Union."

DESY's real mission will not change as a result, Willner emphasises: "At DESY, we will continue to focus on fundamental research, but there's no conflict here with innovation or knowledge transfer – the two sides are interlinked. We're going to be asking how we can take what we already have and make it more easily exploitable and usable by industry." To this end, DESY is networking with industry, partner institutes and policymakers. Concrete measures include providing experimental facilities and know-how, supporting product development and spin-off companies, and setting up an innovation centre in partnership with the University of Hamburg and the City of Hamburg.

At DESY, the innovation process already begins with the construction of complex particle accelerators for research. The requisite components and procedures are based on cutting-edge technology and often demand radical new solutions. These will later find application in fields such as medicine, radar and satellite technology or in chemical processes.

## WHEN INNOVATION LEADS TO REVOLUTION

Sometimes, a scientific discovery can lead quite by chance to a host of innovations and new applications. A classic example is synchrotron radiation, a special type of light produced by particle accelerators. For particle physics experiments, this radiation is merely troublesome interference. Yet as early as the 1950s, a number of scientists recognised its potential. Synchrotron radiation, especially in the X-ray range, is ideal for investigating a host of materials.

It was over 50 years ago that experiments with this intense form of light first began at the DESY ring accelerator. Today, DESY is one of →

In July 2016, Arik Willner took up the newly created position of Chief Technology Officer (CTO) at DESY, where he also heads the Innovation and Technology Transfer office.

# "WE HAVE THIS DYNAMISM"

**femto:** Why are innovations so important for DESY?

**Arik Willner:** I think that a publicly funded research centre must ask itself how it can also benefit society over the short and medium terms by utilising what its scientists discover and develop, and how it can help to solve mankind's most pressing problems.

**femto:** Why is DESY important for industry?

**Arik Willner:** Companies are noticing that they are too slow in the global competition for new ideas if they organise their development departments like high-security labs. That's why the focus is on open innovation. In this process, companies are opening themselves up to research institutes such as DESY and want to get in touch with us. For example, industrial firms have welcomed our initiative to discuss the PETRA IV project. We want to find out what challenges industry faces in the various sectors and how we can address them with PETRA IV. Siemens and Bosch have expressed an interest in working together with us to develop future medical technology and medical imaging systems. Philips, meanwhile, wants to work together with us in a variety of areas. All of these companies face global competition and benefit from including players such as DESY in their innovation chains.

**femto:** What can DESY offer industry?

**Arik Willner:** Our high-tech facilities, our technologies and our know-how. Our X-ray radiation sources PETRA III and FLASH provide companies with great opportunities, as does our supercomputer. Moreover, we are currently creating networks with partners such as the Hamburg University of Technology and the Hamburg University of Applied Sciences (HAW) in order to provide companies with comprehensive support. Companies have to become more dynamic again. We have this dynamism, but haven't thought very much about how we can use it to have an economic and social impact.

**femto:** Does that only benefit the companies?

**Arik Willner:** Everybody has to work together to create a win–win situation for all the partners. In exchange, we learn from industry and get money that we can invest in research. However, the local region benefits as well. In Hamburg, we are deeply involved in the Senate's innovation strategy. Our site is to develop into a research and innovation campus, with focus on the life sciences, nano- and laser technology and new materials. That's our innovation profile. DESY has a lot of methodological expertise and much know-how in this area.

DESY is also involved in Brandenburg's innovation and transfer strategy – not only at our location in Zeuthen, but also through the DESY foundation as a whole, i.e. with all of the innovations we create. We contribute to society's development – in the region, in Germany and in Europe as a whole.

the world's leading centres for research with X-ray radiation from particle accelerators. Using the DESY facilities, scientists are examining diverse materials as well as cultural artefacts, bone implants, nanomaterials and biomolecules, all at the atomic level.

The summer of 1970 was the start of another success story at the DESY accelerator. This was when Ken Holmes and Gerd Rosenbaum used synchrotron radiation to capture the first ever diffraction images of insect wing muscles. It was the birth of structural biology. The pioneers of this nascent discipline then used the DORIS storage ring, commissioned in 1974, to decrypt the molecular processes involved in muscle movement. The intense, highly collimated X-rays from particle accelerators proved ideal for investigating the structure of proteins in detail – and became a genuine driver of innovation. Working at DORIS, the biochemist Ada Yonath would later conduct groundbreaking investigations of the complex structure of the ribosome, one of the key molecules of life. In 2009, she and her two colleagues were awarded the Nobel Prize in Chemistry.

## THE BOOM IN STRUCTURAL BIOLOGY

Today, DESY operates one of the world's top X-ray radiation sources – PETRA III – and offers first-rate experimental facilities for researchers who require highly collimated, very short-wave X-ray light for their work. "Today's X-ray radiation sources enable us to decipher the atomic structure of biomolecules and pathogens and thus systematically investigate how they function. This gives biological research a whole new dimension," explains Matthias Wilmanns, founding director of the Centre for Structural Systems Biology (CSSB), a centre for infection research on the DESY campus. "We're operating a kind of Google Maps for the human body. Mankind has a vital interest in being able to zoom in on the body as closely as possible. Thanks to X-ray structural analysis, we can now observe individual atoms."

This paves the way for new approaches in drug research – for example, in the fight against infectious diseases. "There are around 30 000 proteins in the human body," Wilmanns explains. "The simplest idea for a new drug is to selectively block one of these proteins using a small customised molecule with exactly the right shape. This is often known as the 'lock and key' principle, but in reality it's more like a three-dimensional map with mountains, valleys, craters, caves and lots more. The more we know about these structures, the better we can tailor something to fit them, and the less we have to use trial and error. And instead of the extremely expensive approaches that often have to be adopted in pharmaceutical research, we can take shortcuts and save millions of euros."

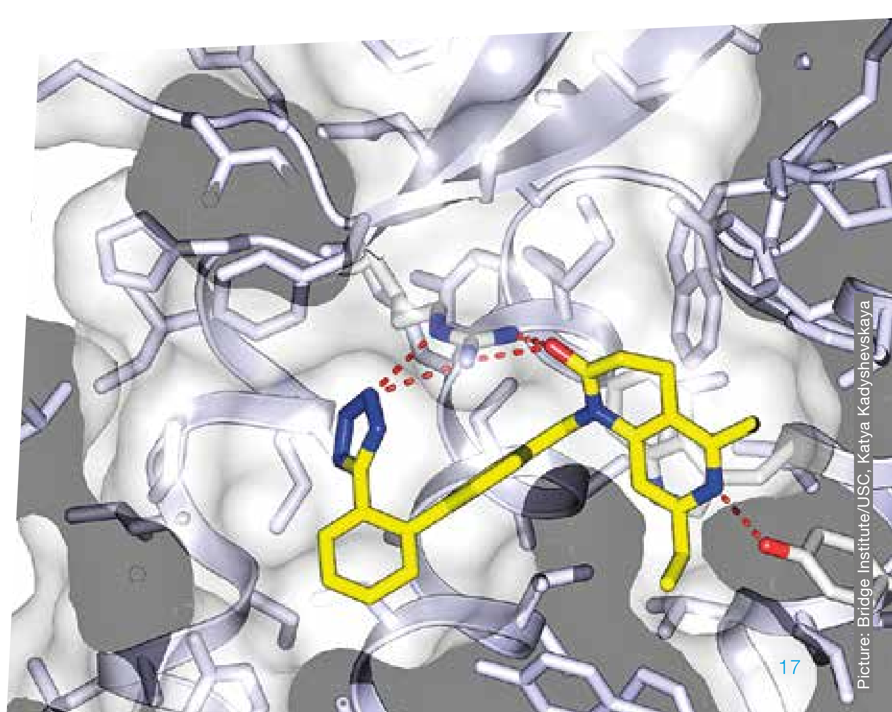
"We're operating a kind of Google Maps for the human body"

MATTHIAS WILMANNS
CSSB

## THE FUTURE IS ANIMATED

Experimentation with synchrotron radiation grew initially out of simple scientific curiosity. Even in their wildest dreams, those first pioneers would never have imagined the almost revolutionary innovations their early work would unleash. While such breakthroughs can never be planned, it is certainly possible to cultivate the ground from which such innovations spring.

Molecular structure of the binding pocket of the blood-pressure regulator AT1R with a bound molecule



Picture: Bridge Institute/USC, Katya Kadyshevskaya

HENRY CHAPMAN
DESY/CFEL

"By arranging these ultrafast snapshots into a film, we can produce a slow-motion sequence of molecular dynamics"

In the field of science, this means providing first-rate experimental facilities and bringing together smart people. At DESY in Hamburg, this has led to the creation of an international and interdisciplinary research campus with unique X-ray radiation sources and a host of partner institutes. In nanoscience and bioscience, for example, it has generated outstanding research opportunities that have already given rise to many innovations. The next revolution in structural research is about to commence in Hamburg with the operational start-up of a new international X-ray laser, the European XFEL. In a field that once relied on still images, it now becomes possible to record atoms and molecules in motion. Chemical reactions, changes in materials, pathogens attacking human cells – all these processes can be "filmed" as they happen, at atomic resolution. Like a flip book, these films are made up of a sequence of snapshots.

X-ray lasers make it possible to capture such images from the nanoworld at a temporal resolution in the femtosecond (quadrillionth of a second) range. "By arranging these ultrafast snapshots into a film, we can produce a slow-motion sequence of molecular dynamics," explains DESY researcher Henry Chapman from the Center for Free-Electron Laser Science (CFEL). Such images shed a whole new light on a range of biochemical processes, including medically relevant processes in the human body and technologically interesting processes in nature.

## GROUNDBREAKINGLY NEW

Fundamental research plays a very special role in the innovation process. Rather than being strictly focused on the immediate exploitability

Picture: DESY, Dirk Nölle

The European XFEL X-ray laser is powered by the world's longest superconducting linear accelerator.

of results, such research lays the foundations for the innovations of the future. Instead of being geared towards optimising something that already exists, this type of research looks to break completely new ground. Yet the two approaches are not mutually exclusive. On the DESY campus, it's not unusual for scientists studying the fundamental evolution of the universe to encounter researchers developing a new form of data storage or budding entrepreneurs looking to base a business model on a new technology.

Developments that offer promising and wide-ranging applications include new nanomaterials, which are being investigated and customised with atomic precision using DESY's X-ray radiation sources. One nanometre is one millionth of a millimetre. Nanostructured matter has different physical and chemical properties than matter with structures on the centimetre or metre scale. This fact has attracted the attention of both science and business, creating a whole new field of research and industry, which is now busy investigating these new phenomena, →

# "Promoting start-ups in Hamburg"

**A guest column by Hamburg's First Mayor Olaf Scholz**

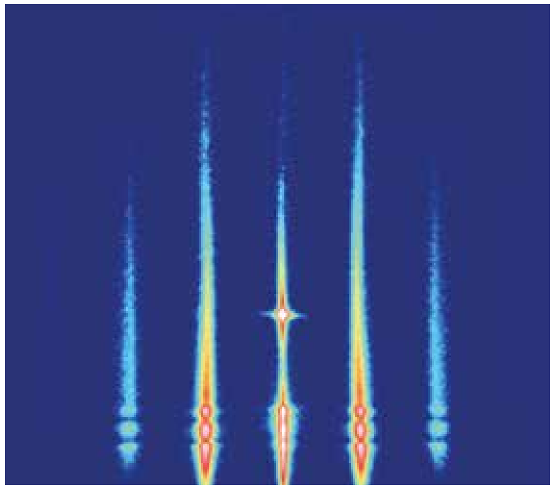
Here in Hamburg, we know how to make knowledge-based structural changes. As a result, the European Commission honoured Hamburg last year as one of Europe's most innovative regions. Our various clusters have received several awards, and Hamburg is also Germany's number one location for start-ups.

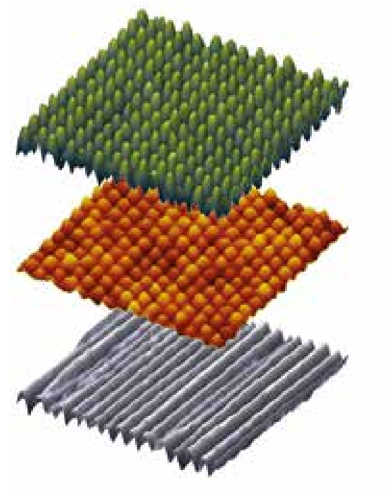
Start-ups in particular need places where innovation occurs. One such place is the innovation centre that will jointly be operated by DESY, the University of Hamburg and the City of Hamburg. The centre will offer an attractive environment for spin-offs, technology start-ups and small businesses that will benefit from the close proximity to DESY. The innovation centre and the planned research and innovation park nearby are an example of how knowledge and innovation can be successfully transferred. With these facilities, we are creating important preconditions for continuously turning innovations into marketable products.

However, Hamburg also promotes the creation of start-ups in many other ways besides the research and innovation park. Research institutes such as DESY, which set scientific benchmarks worldwide, generate lots of ideas for products and thus for companies that are extremely innovative and competitive. These companies operate on international markets or even create them. They generate growth, add value and create high-quality jobs.

In order to promote such start-up ideas, we will strengthen the networks between researchers at the universities and research institutes who can imagine founding their own companies and the bodies promoting the creation of start-ups in Hamburg, and we will establish a platform that will address the special needs of such knowledge-intensive start-ups. Doing so will kick off the further expansion of start-up support at Hamburg's universities and research institutes.

The growth of self-organising nanolayers (right) can be observed under X-ray light (left).





Picture: DESY, Denise Erb/Kai Schlage

properties and the potential applications of structures measuring less than 100 nanometres.

## THE FUTURE IS NANO

"DESY's X-ray sources FLASH and PETRA III are ideal supermicroscopes for observing and understanding structures and processes in the nanoworld," emphasises DESY Research Director Edgar Weckert. "At our Hamburg campus, we work together with various institutions and partners to conduct interdisciplinary research on materials at the nanoscale." The DESY NanoLab combines these radiation sources with a range of analytical equipment and methods so as to investigate materials, nanoparticles, surfaces and processes at the nanoscale and obtain a comprehensive understanding of any potential applications.

For example, DESY researchers have developed a new process whereby metallic nanostructures can be made to line up and assemble themselves all on their own. This bottom-up approach offers a quick and simple alternative to existing procedures, making it also interesting for commercial applications, where nanostructures are increasingly used. New nanomaterials with customised properties are also developed at DESY, including, for example, a new class of material that is hard and has high tensile strength. To develop this material, a research team from DESY, Hamburg University of Technology, the University of Hamburg and Helmholtz-Zentrum Geesthacht combined nanoparticles of iron oxide with a coating of organic oleic acid. Researchers at DESY have also identified a new mechanism that could lead to the development of superhard and supertough ceramics for industrial applications.

"DESY's X-ray sources FLASH and PETRA III are ideal supermicroscopes for observing and understanding structures and processes in the nanoworld"

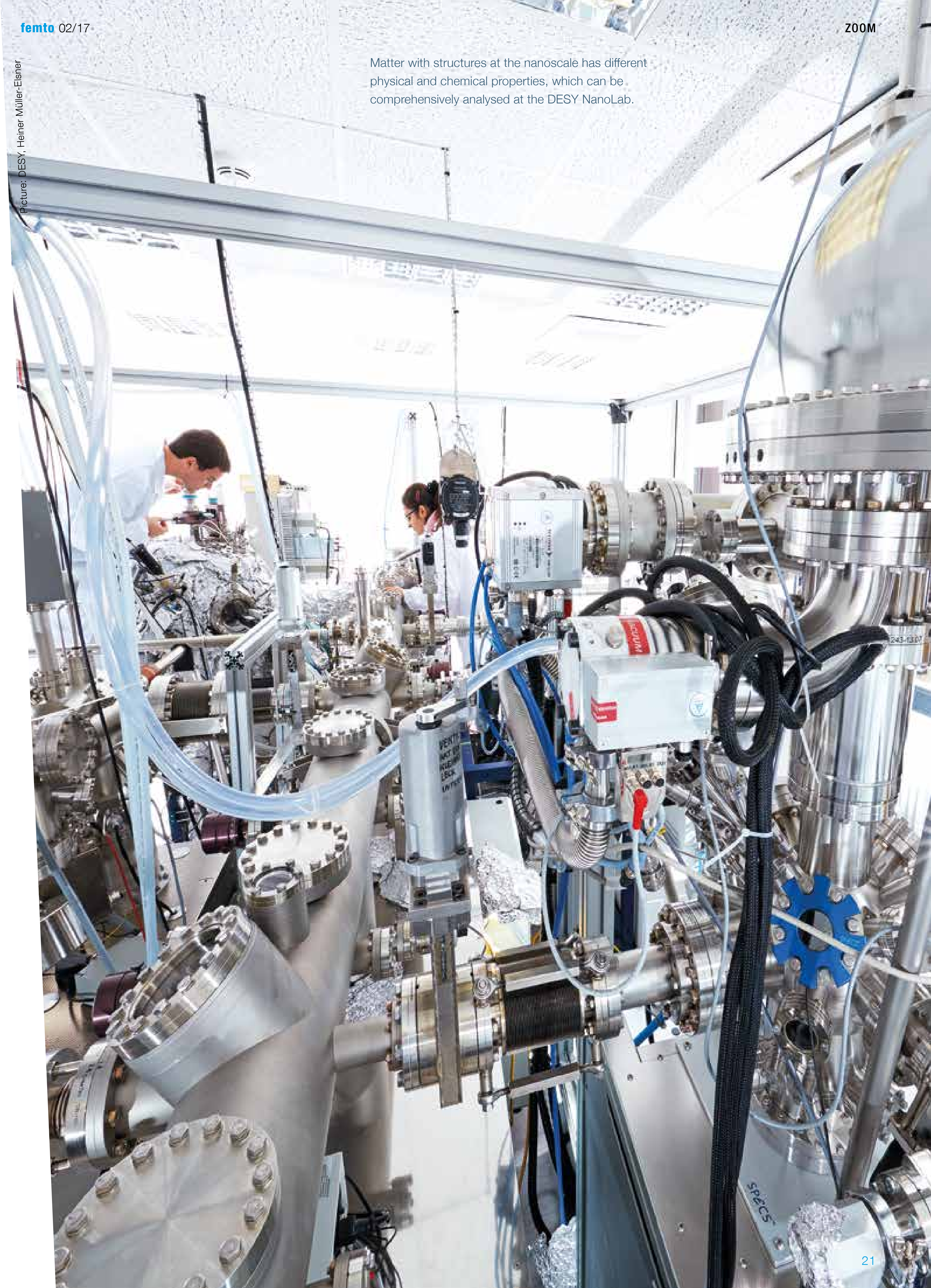
**EDGAR WECKERT**
*DESY*

## LIVE VIEWS OF CATALYST WEAROUT

Also highly promising is the investigation and development of new catalysts. These are materials that accelerate chemical reactions or enable them in the first place. They are indispensable in many industrial processes. The best-known example is undoubtedly the catalytic converter in cars. This system uses a mixture of platinum, rhodium and palladium to convert toxic carbon monoxide and harmful nitrogen oxides into less hazardous compounds. Researchers working at DESY's X-ray radiation source PETRA III have now observed that, under the operating conditions in an automotive catalytic converter, the platinum nanoparticles coalesce and become less efficient. Researchers have also developed a high-speed X-ray technique with which the atomic structure of surfaces can be analysed at a speed that produces live recordings of surface reactions such as catalysis or corrosion with a temporal resolution of less than one second. "We can now investigate surface processes that were once unobservable in real time and which play a key role in many areas of materials science," explains Andreas Stierle, Director of the DESY NanoLab.

Picture: DESY, Heiner Müller-Elsner

Matter with structures at the nanoscale has different physical and chemical properties, which can be comprehensively analysed at the DESY NanoLab.



Picture: DESY, Heiner Müller-Elsner

The MicroTCA.4 electronics standard can be used in a variety of applications, ranging from particle accelerators to aviation.

# THE MicroTCA.4 TECHNOLOGY LAB

In many cases, the development of new particle accelerators leads to technological innovations with great potential for further applications. An example is the required control technology, which has to be very precise, extremely fast and able to process a large of number data sets in parallel. Various electronic standards have been established to facilitate the development of systems capable of meeting such specifications. These provide a uniform description on the basis of which such systems can be constructed. But, as DESY accelerator expert Holger Schlarb points out, "Ultimately, none of the standards was suitable for DESY's future development." For this reason, Schlarb and his team developed a new industrial standard in cooperation with partners, and worked together with DESY's Innovation and Technology Transfer office to bring it to market maturity.

The team first looked at the standard that most closely approximated their requirements: MicroTCA (Micro Telecommunications Computing Architecture). "This is a very widespread industry standard," Schlarb explains. "It comes from the telecoms sector and does everything we want, except for one thing: recording extremely fine-quality analogue data." DESY physicists therefore collaborated with other institutes and industrial partners to add a range of essential features to the standard. MicroTCA.4 now combines ultrafast digital electronics with the optional integration of analogue components in a very compact format. Its immense reliability and great scalability make it ideal for controlling particle accelerators. There are many potential fields of application in industry as well, including telecommunications, online inspection, aviation, medical engineering and precision metrology.

Last year, DESY teamed up with business partners to create the MicroTCA.4 Technology Lab, which receives public funding as a Helmholtz Innovation Lab. The lab aims to enhance the MicroTCA.4 standard and establish it on a large market. "The MicroTCA.4 Technology Lab is an important building block in the research centre's innovation strategy," says DESY Director Helmut Dosch. "It will open up a new dimension of cooperation between DESY and private enterprise."

## A NEW GENERATION OF SOLAR CELLS

At the measuring stations of PETRA III, work is also under way to investigate solar cells so that they can be improved. These include plastic solar cells with organic semiconductors, which are flexible, formable, lightweight, inexpensive and therefore highly versatile. Moreover, they can be produced in printing processes that save material and energy. However, before these solar cells are ready for market, a number of obstacles must be overcome: Energy conversion efficiency needs to be improved, production cost reduced, and the service life of materials and modules increased. To this end, various groups are carrying out experiments at PETRA III. Advances here include the enhancement of a production process developed by Danish researchers and improvements in performance of the plastic solar cells through the addition of magnetic nanoparticles.

## DESY's INNOVATION ACCELERATOR

It is therefore an exciting time for materials science and medicine. Yet the innovation process starts much earlier, with technical breakthroughs in the development and construction of the research facilities that make such applications possible in the first place. The development of new particle accelerators and detectors is pioneer work and has been the key area of expertise at DESY for over 50 years. Whenever new accelerator or detector technology is devised for particle physics or X-ray research, DESY is one of the leading players worldwide. For example, DESY

femtopolis

# Meeting up for a cup of coffee...

To start off – tea of course works just as well. What we're interested in here is the social function of mankind's favourite drinks. "Should we meet up for a cup of coffee?" It's a classic lead-in for starting a conversation, getting to know one another or sharing ideas. Beverages help promote social interaction in private life as well as in professional situations. During the Age of Enlightenment, Europe's coffee houses served as important places for exchanging news and initiating business deals. Today, companies are setting up coffee corners and tea rooms so that employees feel at home, share knowledge and ultimately become more productive. Communication areas are also very important in state-of-the-art research buildings, where coffee and other beverages are a must to achieve the desired unifying effect.

Ideally, outstanding researchers from a variety of scientific disciplines meet here to talk shop about the optimal preparation of a latte macchiato or are annoyed about the thin crema on the espresso before being surprised to find out that the person they are talking to has developed a method that could help them make major progress with their own research project. People need other people in order to discover their abilities, disentangle complex knots and achieve truly brilliant solutions. Coffee is good for promoting such interaction. By definition, coffee is a hot, black, psychotropic beverage that contains caffeine and is made from roasted ground coffee beans and hot water. Moreover, it is the most popular beverage in Germany. That coffee breaks have a positive effect has been scientifically proven. Studies have shown that such breaks increase a person's productivity and ability to concentrate while at the same time reducing stress.

Coffee breaks have now even become a distinctive conference format. As the Irish publisher and software developer Tim O'Reilly found out, participants at traditional conferences actually benefited the most from the coffee breaks. As a result, O'Reilly came up with the "unconference" concept. Instead of imparting knowledge in classroom-like presentations, the concept promotes the exchange of ideas between the participants. In 2005, he initiated the first Foo ("Friends of O'Reilly") Camp in Palo Alto, California – an *ad hoc* event where the participants organised the content and schedule themselves.

Today, such unconferences (also known as "bar camps") are a well-established format, with open-space meetings offering a lot of design freedom and interaction. But no matter whether bar camp or traditional conference: Coffee is a must at all types of meetings.

New methods for handling the big data generated by research are continually being developed at the DESY computer centre.

Picture: DESY, Heiner Müller-Elsner

is strongly involved in development work for the Large Hadron Collider (LHC) – a veritable "world machine" – at the CERN research centre near Geneva.

Another prime example is the European XFEL X-ray laser. Eleven countries are participating in this international project. DESY is the main shareholder and is responsible for the construction and operation of the facility's linear accelerator. The superconducting technology for the accelerator was developed in an international collaboration led by DESY. "The accelerator is an outstanding example of successful global cooperation involving not only research facilities, institutes and universities but also companies from industry that have produced individual components," says Robert Feidenhans'l, Chairman of the European XFEL Management Board. Superconducting means that the accelerator components operate without any electrical resistance. For this, they have to be cooled to an extremely low temperature. The companies involved in the project also profit from the developments and breakthroughs in building such a high-tech facility. The know-how they gain in the manufacturing process gives them a vital technological edge.

> "The accelerator is an outstanding example of successful global cooperation involving not only research facilities, institutes and universities but also companies from industry that have produced individual components"

**ROBERT FEIDENHANS'L**
*European XFEL*

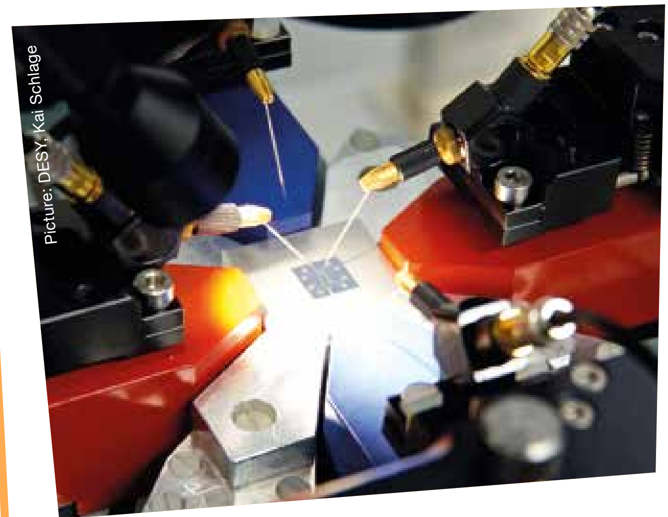
## THE AGE OF BIG DATA

Large particle accelerators generate massive amounts of data, which must be analysed and stored. For this reason, particle physics has always been a key driver of innovation in the field of computer technology. Today, the huge volumes of data produced in diverse scientific fields have themselves become the object of new research. The sensors, special cameras and detectors used by researchers to observe their experiments are becoming more and more powerful. They supply higher resolutions, sharper images and faster readings – and thereby ever greater volumes of data in ever shorter times. But this also means that it is getting more and more difficult to transfer, store and analyse this data. "The old techniques are no longer fit for purpose," says Volker Gülzow, head of IT at DESY. "We need new methods."

That means, on the one hand, innovative concepts for hardware and software to capture and reliably store the data and, on the other, fast algorithms and sophisticated computer programs to analyse the readings. Advances in this area include a technology known as dCache – a system for the intelligent administration of huge data volumes developed by DESY in collaboration with the US research centre Fermilab and the Nordic Data Grid Facility. The storage facilities of today's data grids have to be capable of not only accommodating this flood of data but also ensuring it can be accessed from anywhere around the world. "dCache automatically shifts data between different storage media such as

hard disk and magnetic tape, depending on what is most practical for the user," explains project leader Patrick Fuhrmann from DESY. "The system acts like a cache, ensuring that the data are constantly available for computing purposes, irrespective of where they come from." Today, this system is used not only for the data produced by the LHC but also for other scientific areas – as well as by businesses such as banks.

Science has a manifold impact on society's potential to innovate. Ultimately, this is the case wherever research or development takes place. In industry, by contrast, the focus is narrower: An idea first becomes an innovation when it has developed into a marketable product or service and is generating a profit. When applied to DESY, as CTO Arik Willner explains, this means that "in order to speak of innovation, we have to have an impact on industry and on society. That might mean generating a profit for a company or having an impact on a regional business strategy." →




The novel magnetic sensors can be adapted to a wide variety of applications.

# MAGNETIC SENSORS FOR INDUSTRY

Magnetic sensors – or, more correctly, magnetoresistance sensors – are tiny, extremely sensitive high-performance helpers in our daily lives. In cars, they measure the rotational speed of the wheels for the ABS braking system and the Electronic Stability Program, or ESP. They are also found in every mobile phone, read data on hard discs and improve safety by detecting microscopic fractures in metal components. Because of this broad range of applications, the sensors need to operate in a correspondingly customised manner.

The sensors consist of microstructured stacks of alternating magnetic and non-magnetic layers that are only a few nanometres thick. The application of an external magnetic field causes the stack's electrical resistance to change. In 2007, Albert Fert and Peter Grünberg won the Nobel Prize in Physics for the discovery of this giant magnetoresistance (GMR) effect. Although this effect has revolutionised sensor systems, one problem remains: The strength of the magnetic field at which the resistance switches is more or less fixed.

Researchers at DESY have now developed a manufacturing process that enables producers for the first time to control the magnetoresistive properties of the sensor layer systems. The procedure allows the magnetic field strength at which the electrical resistance changes to be flexibly and precisely set in each individual magnetic layer of the tiny stack. In addition, it enables the magnetically preferred direction of the individual layers to be oriented as desired with respect to one another. As a result, producers can easily create a wide range of new sensor properties.

"Until now, applications often had to be adapted to the sensors. Our technique, however, enables us to tailor sensors to the desired application," says DESY researcher Kai Schlage. Money from the Helmholtz Validation Fund is being used to develop the sensors to the commercial market stage. To this end, the sensors are being tested in industrial environments, for example, in order to ensure that they meet the requirements of the automotive sector and other areas of application.

Picture: DESY, Gesine Born

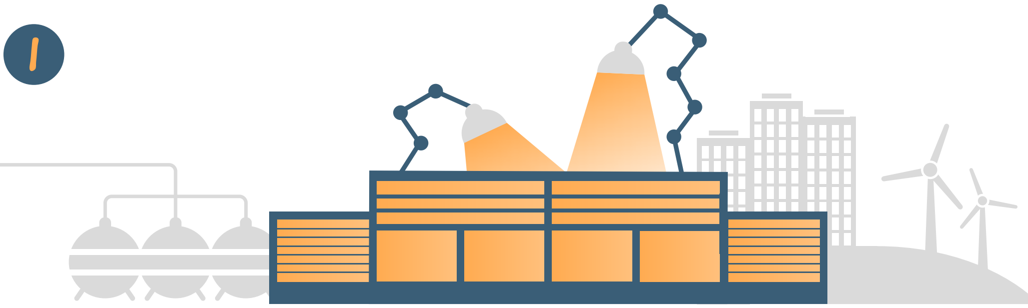
Christian Schroer is the scientific head of the X-ray radiation source PETRA III.

# AN X-RAY MICROSCOPE FOR NANORESEARCH

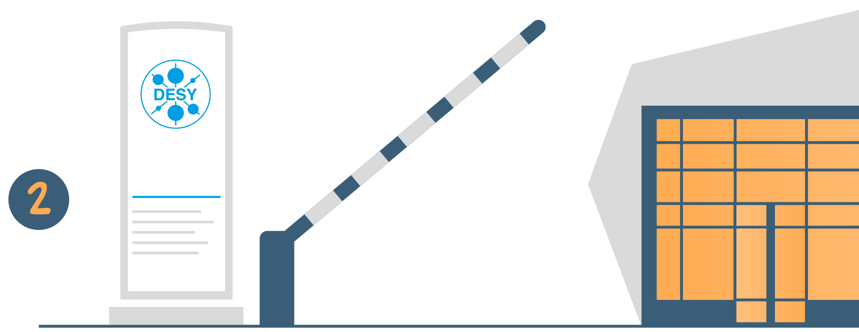
At its Hamburg campus, DESY operates one of the world's best storage ring X-ray radiation sources: PETRA III. Research groups from around the world use its intense X-ray radiation, which is especially brilliant, for a host of experiments ranging from medical research to nanotechnology. Yet the 2300-metre-long ring accelerator holds even greater potential. The facility could be extended to create an extremely focused, high-resolution 3D X-ray microscope, which would open up outstanding research opportunities for the future-oriented nanosciences and materials sciences.

Under the project name PETRA IV, DESY is planning to create such an ultimate X-ray microscope, which would enable researchers to investigate the physical and chemical processes inside materials at all scales, from a few millimetres to atomic dimensions. Processes that occur at the molecular level in catalysts, batteries or microchips could be analysed under realistic operating conditions, while the properties and processes in promising new materials could be understood and controlled in order to create tailor-made materials with nanostructures.

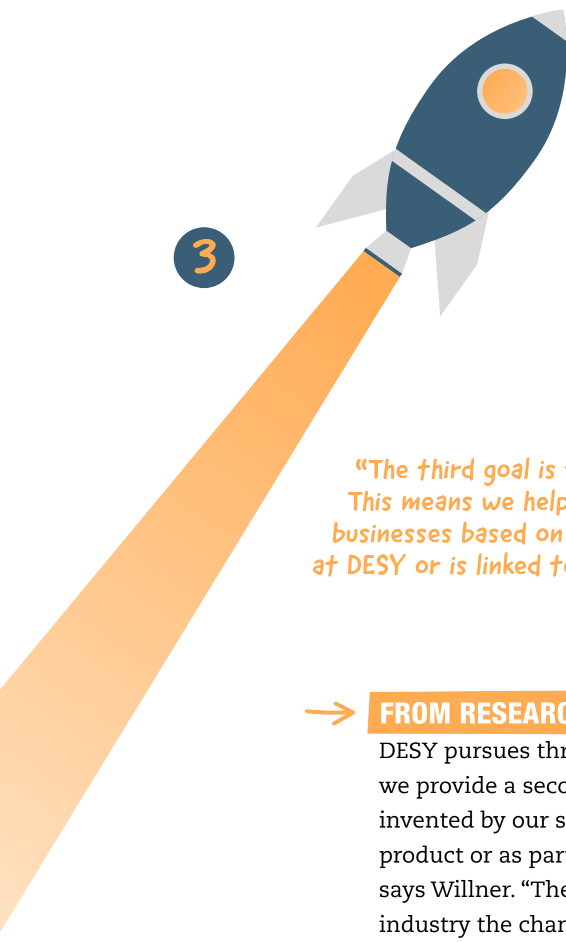
"These new experimental opportunities will help industry lay the foundations for the development of new production processes and new materials," says Christian Schroer, the facility's leading scientist. "For example, it will be possible to follow on the nanoscale what happens at specific locations inside a battery during the normal charge and discharge processes. We will be able to see how and why it ages and to develop ways of preventing this. The same applies to a whole range of material samples – in the field of aircraft construction or lightweight engineering, for example, where we will be able to follow, at atomic resolution, exactly what happens when such materials are produced and as they wear."




"The first goal is that we provide a second use for the technologies invented by our scientists, namely as a market product or as part of industrial machinery"




"The second goal is that we offer industry the chance to use our know-how and our facilities and instruments, all of which are unique, thereby helping companies to bridge gaps in the innovation chain"




"The third goal is that we support spin-offs. This means we help our scientists to set up their own businesses based on technology that either was developed at DESY or is linked to DESY patents"

## FROM RESEARCH TO INDUSTRY

DESY pursues three goals here. "The first is that we provide a second use for the technologies invented by our scientists, namely as a market product or as part of industrial machinery," says Willner. "The second is that we offer industry the chance to use our know-how and our facilities and instruments, all of which are unique, thereby helping companies to bridge gaps in the innovation chain. And the third is that we support spin-offs. This means we help our scientists to set up their own businesses based on technology that either was developed at DESY or is linked to DESY patents."

DESY has already helped launch a number of highly promising high-tech spin-off companies. These include Class 5 Photonics GmbH, which was set up by DESY and the Helmholtz Institute Jena. The company develops high-performance lasers for science and industry. In another example, a team from the DESY detector development group devised a fast high-resolution X-ray camera by the name of LAMBDA and set up the company X-Spectrum GmbH on this basis. The DESY spin-off suna precision GmbH sells innovative measuring instruments based on new nanopositioning systems, in particular to the scientific market. The company Cycle GmbH arose from work done at DESY's Center for Free-Electron Laser Science (CFEL). This spin-off markets innovative products based on ultrashort-pulse laser technology for both scientific and industrial applications.

## A NEW START-UP CENTRE

In future, budding entrepreneurs from the scientific community will benefit even more from the expertise and infrastructure on →

Picture: DFZ Architekten


The innovation centre will support budding entrepreneurs from the research community.

offer at the DESY campus in Hamburg. Together with the University of Hamburg and the City of Hamburg, DESY is to open a new innovation centre on its research campus. Spin-off companies from DESY, the University of Hamburg or other research institutes will profit from an excellent location featuring a unique combination of office and laboratory space. Start-up companies from elsewhere will also be able to rent space here. The new innovation centre, which is to be built on a site of some 5000 square metres in the immediate vicinity of the research facilities on the DESY campus, is scheduled to be ready for occupancy in 2019.

# INNOVATION GLOSSARY

### Innovation

Literally, making anew or renewal, from the Latin verb innovare, to renew. In a strict sense, an innovation first arises when an idea has been translated into a new product, service or process that has become widely adopted and successfully established on the market.

### Innovation hacking

Innovation hacking means that new ideas are no longer researched, developed and analysed to the finest detail but rather tried out and brought to market in small test batches as quickly as possible. The advantage is that it quickly becomes clear what works and what doesn't. That way, the original idea can be improved or enlarged, thereby limiting the risk during a long development process that the competition might happen upon the same idea and then claim it as their own.

### Design thinking

Design thinking is an approach geared towards solving problems and developing new ideas. The aim is to find solutions capable of convincing the customer. Design thinking presupposes that problems are more readily solved when people from different disciplines work together creatively and develop concepts that are tested a number of times.

### Disruptive innovation

An innovation is characterised as disruptive when it changes the rules of the game either on the market or in user behaviour. This is also known as a revolutionary innovation and differs from evolutionary or incremental innovation, whereby an existing technology or product is enhanced, made more efficient or reduced in price. Design thinking is regarded as a method for systematically producing disruptive innovations or at least making their emergence more likely.

### Open innovation

Open innovation means that the traditionally closed form of the innovation process is opened up to input from outside the company. Here, internal and external ideas alike flow into the development of new products, services and business models. The basic prerequisite for the implementation and use of open innovation is an openness to the ideas of others and a willingness to share one's knowledge with them.

NICK SOHNEMANN
*Future Candy*

ANDREAS RINGWALD
*DESY*

# "WE ARE LIVING IN AN AGE IN WHICH INVENTORS AND PIONEERING THINKERS ARE GREATLY APPRECIATED ONCE AGAIN"

Every innovation begins with an idea – one that is so good that it can be turned into something completely new. But how does one come up with such ideas? And how are these ideas transformed into innovations? These issues are discussed here by physicist Andreas Ringwald, who is investigating the big mysteries of the universe in theoretical particle physics, and innovation consultant Nick Sohnemann, who founded the agency Future Candy and helps businesses become more innovative.

**femto:** In most cases, you don't simply sit at your desk and plan to have an idea...

**Andreas Ringwald:** The ideas actually come spontaneously. For example, I get ideas when I relax while sailing and try not to think about anything. But of course you can't stop thinking. I then write down the ideas I get in the logbook. As scientists, we don't consider whether we want to be innovative or not. Instead, we have questions that we want to answer.

**Nick Sohnemann:** It's more or less the same at our company as well. Businesses are currently falling into a kind of hypercompetition. Innovations produce only short-term benefits. That's why innovation is now an ongoing topic. The far-reaching digital transformation of the economy is making the new era unpredictable. The only thing you can do is to create new concepts, try them out and quickly develop a prototype.

**Andreas Ringwald:** Does that mean one shouldn't make any plans? Does innovation simply happen without any planning?

**Nick Sohnemann:** Not quite, but planning work is no longer as rigid and time-consuming as it used to be. In the six months that it takes me to analyse the ideas from my development department and select some of them for further consideration, so many new things happen. I have to continuously observe how the market is developing. I have to find out what works for my customers. And I have to look at my corporate culture to find out what works with my employees.

**femto:** What is the very first step in the innovation process?

**Nick Sohnemann:** For us, the first step is the customer. We have internalised all of the new methods from Silicon Valley, such as design thinking and lean start-up, adapted them to the German market and used them as the basis for developing our innovation hacking process. All of these methods always begin with an understanding of the customer so that you can engage in customer-focused innovation.

**femto:** What does this mean?

**Nick Sohnemann:** A familiar example is the fact that people don't want drills, they want a hole in the wall. Another example is that I want to have groceries, but not have to go to the supermarket. And I want to get to work, but not have to drive myself. Can technology help me do all that? On the basis of such findings, we begin to come up with ideas.

**Andreas Ringwald:** I begin with the big questions that we address in fundamental research. Physicists already have certain approaches that they use to solve specific problems. I always try to find something that combines the various approaches into an overarching theory, so that the questions all fit together in the grand scheme of things and can be resolved.

**femto:** So the process is more evolutionary than revolutionary?

**Andreas Ringwald:** As far as I can see, there aren't any completely new approaches at the moment. My approach is to combine a vast number of different pieces, like in a puzzle. To do that, you have to research a variety of different topics or you won't be able to complete the puzzle.

**Nick Sohnemann:** It's the same with us. There are always counter-developments to trends – such as a focus on the senses instead of technology. There are many new business models and platforms that we need to keep an eye on. In the 1980s and 1990s, consultants told companies to focus on their core business and cut back in other areas. Today, this core business approach has turned many big companies into bad innovators because they always think that they must focus on a single thing – whatever it is they have the most experience in.

**femto:** And how do you help such companies?

**Nick Sohnemann:** We are like a creative agency for innovations. Companies ask us to transform their corporate cultures. In many cases, this transformation process first moves inward. All of the employees have to be convinced to support the strategy and the innovation processes. We can see that things are changing so fast that forecasts and plans can quickly become obsolete. The only thing that helps here is to try out new ideas. The new products are different from those of the old economy.

**Andreas Ringwald:** I didn't really expect you to say that. Whenever I hear about innovation, it generally sounds like planned economy. When I started to work in physics, I never planned in advance what I wanted to find out. Instead, I read research texts, stumbled on new developments and did things. In fact, I mostly do things that nobody else does. However, I can't plan what problems I will be working on over the next five years.

**femto:** Is science hampered by too much planning?

**Andreas Ringwald:** That depends on the field you are working in. The big LHC experiments involving thousands of people have to be planned in advance, of course, but such planning could be rather counterproductive in theoretical physics. For example, I applied for a project at the German science and research organisation DFG (Deutsche Forschungsgemeinschaft). One week after everything was written and approved, I discovered something very fascinating and wanted to completely change the project's focus. To my great delight, I was able to do so. We don't always have to rigidly stick to plans, but we need good reasons to deviate from them.

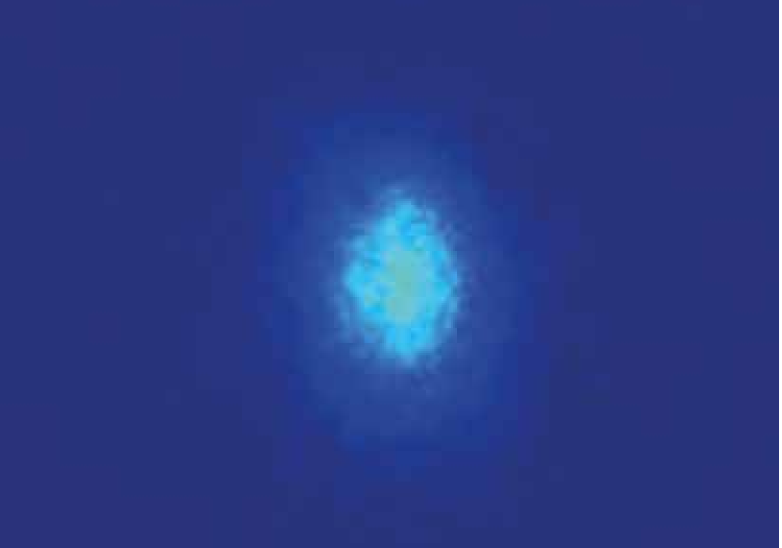
**Nick Sohnemann:** In fundamental research, you probably have much more leeway to try out new things in a trial and error approach. This tends to achieve major breakthroughs more often than is the case in contract research, where processes are optimised step by step.

**Andreas Ringwald:** The DFG now provides funding for "high risk, high gain" experiments.

**femto:** Is innovation something that can make society as a whole fitter for the future?

**Nick Sohnemann:** Yes, it certainly can. We are living in an age in which inventors and pioneering thinkers are greatly appreciated once again. Many areas are being reshaped as a result of digitalisation. We could contribute to this process. Unfortunately, Germany has few visionaries and hardly any early adopters, who like to buy and try out the latest products. They are more prevalent in Silicon Valley. However, Germans are pragmatic, we are something like good second movers. We eventually get on board and then take off!

First laser light at the European XFEL, recorded by an X-ray detector at the end of the tunnel



Picture: DESY

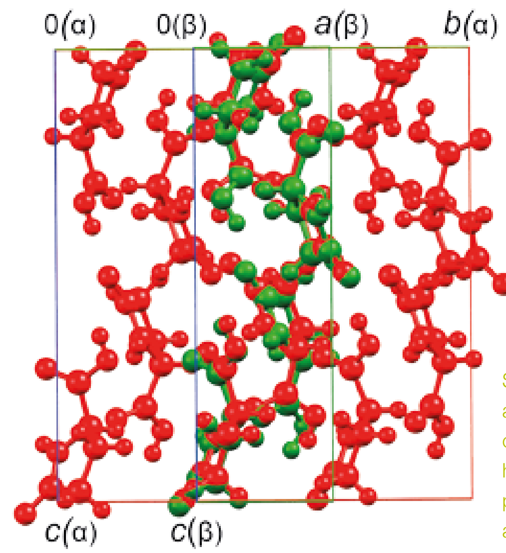
# First laser light

The European XFEL X-ray laser has generated its first laser light. At the beginning of May, the operating team successfully managed the so-called first lasing, with the European XFEL delivering one X-ray flash per second. In the future, this repetition rate will increase to 27 000 pulses per second.

"The European X-ray laser has been brought to life," said Helmut Dosch, Chairman of the DESY Directorate. "The first laser light produced today with the most advanced and most powerful linear accelerator in the world marks the beginning of a new era of research in Europe."

The X-ray light will enable researchers to gain unique insights into the nanocosm, in order to decipher the atomic structure of proteins, for example, or to film chemical reactions in atomic super slow motion. Since the official start of the operating phase in early July, first experiments have been possible at Europe's new X-ray laser.

The European XFEL generates its intense X-ray flashes through high-energy electrons from a superconducting particle accelerator, built over the past seven years by a consortium of 17 research institutions led by DESY. The 3.4-kilometre-long X-ray laser runs from the DESY site in Hamburg to the neighbouring town of Schenefeld in Schleswig-Holstein. DESY is the principal shareholder of the European XFEL, which is a joint project of 11 partner countries.




Structure shift in a thermosalient crystal: Upon heating, the position of the atoms shifts from red to green.

Picture: New York University Abu Dhabi, Manas K. Panda/Panče Naumov

# Jumping crystals

Scientists have been fascinated by thermosalient crystals for some time: When placed on a hotplate, these inconspicuous crystals suddenly propel themselves upwards, leaping to heights several times their own length. This abrupt movement is caused by a change in the structure of the crystals. A detailed examination of this transition is very difficult because it is so rapid. An international team of researchers led by Panče Naumov from the New York University Abu Dhabi of the United Arab Emirates has now resorted to a new technique and discovered that immediately before altering their structure the crystals emit a sound wave, the analysis of which revealed further details about the phase transition. In addition, the scientists studied the change in the crystal structure very carefully at DESY.

The phase change and the subsequent movement of the crystals are based on an exciting mechanism: Thermal energy, that is heat, is transformed into mechanical kinetic energy. This energy conversion in the crystals could be of interest for a range of applications. "Such materials could perhaps be used as temperature sensors one day. The phase transition always occurs at a very specific temperature, at which the sensor flips, so to speak," explains DESY scientist Martin Etter. "Another conceivable application is that of converting heat into electricity; but we are still a long way from achieving this."

*Angewandte Chemie, 2017;*
*DOI: 10.1002/ange.201702359*

# New centre for infection research


Ceremonial hand-over of the key: Schleswig-Holstein's Scientific Senator Oliver Grundei, DESY Director Helmut Dosch, Bärbel Brumme-Bothe from the Federal Ministry of Education and Research, CSSB's Scientific Director Matthias Wilmanns, Lower Saxony's Minister for Science Gabriele Heinen-Kljajić and Hamburg's First Mayor Olaf Scholz (from left)

The Centre for Structural Systems Biology (CSSB), a new interdisciplinary infection research centre, has been officially inaugurated on the DESY campus. "The grand opening of CSSB is a milestone for interdisciplinary infection and resistance research," said Olaf Scholz, the First Mayor of the Free and Hanseatic City of Hamburg. "Here, the scientist have access to European-wide unique light and X-ray sources and therefore the chance to combine structural, infection and systems biology – thus creating in Hamburg a novel research focus that places the complex processes and interactions between pathogens and their hosts in the limelight."

The new CSSB building will also provide scientists with direct access to DESY's X-ray light source PETRA III and to the nearby European XFEL free-electron laser. The building's basement was especially designed for the installation of five electron cryo-microscopes, which will enable CSSB scientists to visualise pathogens at various scales of resolution and complexity.

The construction of the building was financed by the Federal Republic of Germany, the Free and Hanseatic City of Hamburg, the Federal State of Lower Saxony and the Federal State of Schleswig-Holstein.

# Tuberculosis infection


Tuberculosis requires an active type-VII secretion system, which is present in many mycobacteria

An international team of scientists has come one step closer to understanding how tuberculosis bacteria infect human cells. The researchers unravelled the molecular structure of a membrane channel that plays a key role in the infection. The team, which included scientists from the Hamburg unit of the European Molecular Biology Laboratory (EMBL) and from the new Centre for Structural Systems Biology (CSSB), both on the DESY campus in Hamburg, presented the first molecular structure of the type-VII secretion system of mycobacteria such as *Mycobacterium tuberculosis*.

"These results represent a big step forward in our understanding of how some of the deadliest pathogenic bacteria such as *Mycobacterium tuberculosis* function," says Matthias Wilmanns, the Head of EMBL Hamburg and the Scientific Director of CSSB. "Our ambition is to use this as a basis to investigate secretion as a mechanism by which mycobacteria infect and interact with the human host." New drugs are urgently needed in the fight against tuberculosis as the bacteria responsible for the disease becomes increasingly resistant to current antibiotics.

Single-particle electron microscopy analysis conducted by the group of Thomas Marlovits at the Research Institute of Molecular Pathology (IMP) in Vienna revealed that the type-VII secretion system is comprised of four types of proteins that form a hexameric ring around a central pore. The system also has flexible molecular "arms" that reach into the interior of the bacterial cell and grasp the molecules that need to be transported.

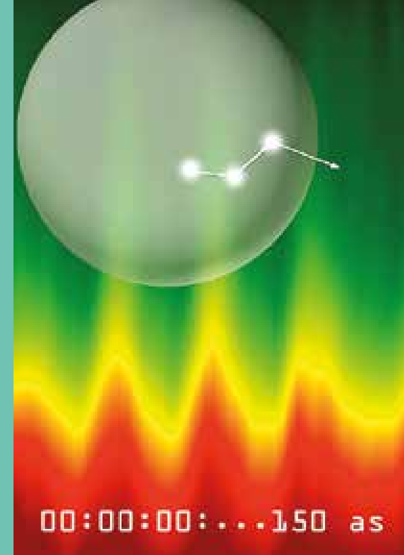
*Nature Microbiology, 2017; DOI: 10.1038/nmicrobiol.2017.47*

# Turmoil in the atomic compound

Electrons in non-conducting materials can be referred to as "sluggish". Typically, they remain fixed in one location, deep inside these atomic compounds. It is hence relatively still in the dielectric crystal lattice. This idyll has now been heavily shaken up by a team of physicists who managed for the first time to directly observe the interaction of light and electrons in a dielectric – i.e. non-conducting – material on timescales of attoseconds (billionths of a billionth of a second).

The scientists beamed light flashes lasting only a few hundred attoseconds onto a 50-nanometre-thick glass particle, which released electrons inside the material. Simultaneously, they irradiated the glass particles with an intense light field, which caused the electrons to oscillate. As a result, the electrons collided with the atoms in the glass. "In an elastic collision, analogous to billiard, the energy of the electrons is conserved, while their direction can change. In an inelastic collision, the atoms are excited and part of the kinetic energy of the electrons is lost. In our experiments, this energy loss leads to a depletion of the electron signal that we can measure," explains Francesca Calegari (CNR-IFN Milan, CFEL-DESY and University of Hamburg).

The researchers' findings could benefit medical applications. With these worldwide first ultra-fast measurements of electron movements inside a non-conducting material, the scientists have obtained important insights into the interaction of radiation with a type of matter that shares similarities with human tissue regarding its dielectric properties.

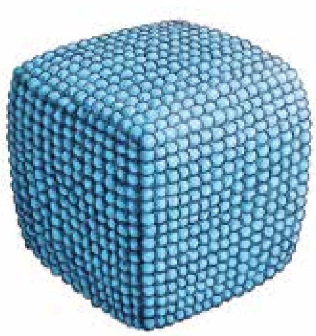



After excitation with ultraviolet light, it takes the electrons 150 attoseconds to leave the dielectric.

Picture: CNR-IFN/CFEL-DESY/University of Hamburg, Francesca Calegari

*Nature Physics, 2017; DOI: 10.1038/nphys4129*

# Vesicle origami



Picture: Moser Graphic Design

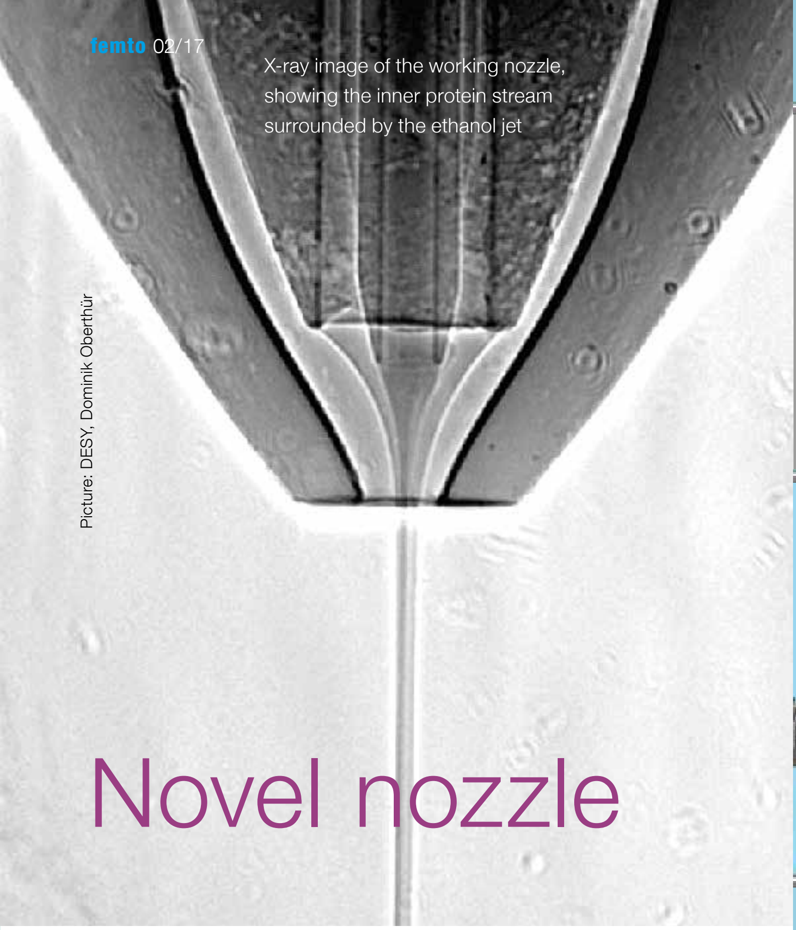
Artist's impression of the observed phospholipid cubes. The molecules are so closely packed that the membrane can scarcely be bent, resulting in the cuboid shape.

For the first time, scientists have observed a phosphorus-containing lipid molecule that self-assembles to form cubes. Research carried out at facilities including DESY has shown that the unusual shape is due to special bonds in the synthetic molecule, a particular phospholipid. Phospholipids play an important role in living organisms, forming cell membranes, among other things. The new findings enhance the understanding of the forces acting within biological membranes and could open up new pathways in medicine, as the researchers headed by Andreas Zumbühl from the University of Fribourg in Switzerland report.

Its unusual structure could make this phospholipid interesting for delivering drugs to specific parts of the body, for example. "The edges of the cube are formed by the outer molecular layer, whereas the inner layer has a discontinuity here. This membrane defect means that the structure may break there if the cube is shaken," explains Zumbühl. A drug that has been encapsulated in the cube can therefore be released in a controlled fashion. "One might for example encase a drug that dissolves blood clots and use this in an emergency after a heart attack. High shear stresses would be exerted on the cube in a blocked artery, releasing the drug at precisely the location where it can do the most good," says Zumbühl.

The cube currently being studied is not itself suitable for such applications, however, since it is as yet too fragile.

*Angewandte Chemie, 2017;*
*DOI: 10.1002/ange.201701634*



X-ray image of the working nozzle, showing the inner protein stream surrounded by the ethanol jet

Picture: DESY, Dominik Oberthür

# Novel nozzle

Thanks to an innovative nozzle, scientists can now analyse more types of proteins while using fewer of the hard-to-get protein crystals. In serial X-ray crystallography experiments, which enable the spatial structure of proteins to be determined in atomic detail, the nozzle can reduce protein consumption eightfold, as the team of inventors headed by DESY scientist Saša Bajt from the Center for Free-Electron Laser Science (CFEL) report.

Biologists are interested in the spatial structure of proteins because it reveals much about the workings of these biomolecules. X-ray crystallography is the prime tool for such investigations. However, it requires crystals of the proteins under investigation, which are then illuminated with X-rays. “Growing protein crystals is complex, the amount of protein that can be produced is often limited to a few millionths of a gram and often only very tiny crystals can be obtained,” says Dominik Oberthür from DESY, the main author of the report.

Using the extremely bright flashes of X-ray free-electron lasers, even those microcrystals can be analysed. To this end, a continuous stream of microcrystals is sent through the pulsed laser beam. Still, even those microcrystals are hard to grow. Bajt’s team therefore devised a new concept for a so-called double flow-focusing nozzle (DFFN) that greatly reduces protein crystal consumption.

*Scientific Reports, 2017; DOI: 10.1038/srep44628*

## femtomenal

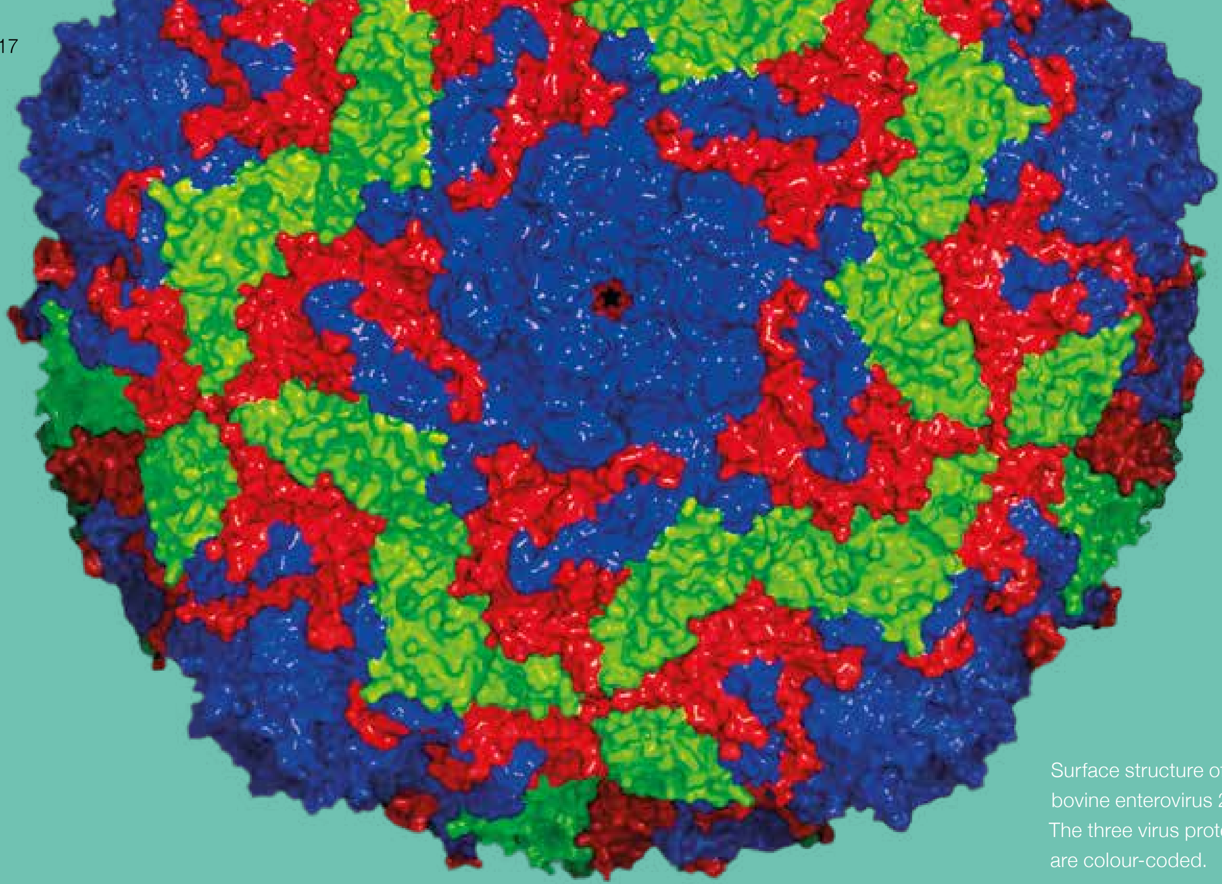

Picture: BioXFEL, Fiacre Kabayiza

The spatial structure of

# 118 814

biomolecules has been decoded to date by means of X-ray radiation. These include many essential proteins that can also serve as starting points for new drugs. The technique of X-ray crystallography, which is used for this purpose, can be demonstrated on smartphones, thanks to the free app XFEL Crystal Blaster (for iPhone, Android, Mac and PC) from the US research consortium BioXFEL. In the app, users shoot an X-ray laser beam at biomolecule crystals such as rhodopsin (also known as “visual purple”) to determine their structure. Each successful hit produces a diffraction pattern that adds to the data set. After enough data has been collected, the protein structure and function are revealed.

**https://www.bioxfel.org/knowledge-transfer/234-xfel-educational-game**



Picture: University of Oxford, Jingshan Ren

Surface structure of the bovine enterovirus 2. The three virus proteins are colour-coded.

# Virus in the X-ray laser

## New method enables analysis in atomic detail

An international team of scientists has for the first time used an X-ray free-electron laser to unravel the structure of an intact virus particle on the atomic level. The method used dramatically reduces the amount of virus material required, while also allowing the investigations to be carried out several times faster than before.

In the field known as structural biology, scientists examine the spatial structure of biomolecules in order to work out how they function. This knowledge enhances our understanding of the fundamental biological processes taking place inside organisms, such as the way in which substances are transported in and out of a cell, and can also be used to develop new drugs. "Knowing the three-dimensional structure of a protein gives unique insight into its biological behaviour," explains David Stuart, Director of Life Sciences at the synchrotron facility Diamond Light Source in the UK and a professor at the University of Oxford, who was involved in the study. "One example is how understanding the structure of a protein that a virus uses to 'hook' onto a cell could mean that we're able to design a defence for the cell to make the virus incapable of attacking it."

X-ray crystallography is by far the most prolific tool used by structural biologists and has already revealed the structure of thousands of biomolecules. To this end, tiny crystals of the protein of interest are grown and then illuminated using high-energy X-rays. The crystals diffract the X-rays in characteristic ways so that the resulting diffraction patterns can be used to deduce the spatial structure of the crystal – and hence of its components – on the atomic scale. However, protein crystals are nowhere near as stable and sturdy as salt crystals, for example. They are difficult to grow, often remaining tiny, and are easily damaged by the high-energy X-rays.

"X-ray lasers have opened up a new path to protein crystallography, because their extremely intense pulses can be used to analyse even extremely tiny crystals that would not produce a sufficiently bright diffraction image using other X-ray sources," adds Armin Wagner from the Diamond Light Source. However, each of these microcrystals can only produce a single diffraction image before it evaporates under the effect of the incident X-ray pulse. To perform the structural analysis, though, hundreds or even thousands of diffraction images are needed.

In such experiments, scientists therefore inject a fine liquid jet of protein crystals into the beam of a pulsed X-ray laser, which delivers a rapid sequence of extremely short X-ray flashes. Each time an X-ray pulse happens to strike a microcrystal, a diffraction image is produced and recorded.

This method is very successful and has already been used to determine the structure of more than 80 biomolecules. However, most of the sample material is wasted. "The hit rate is typically less than two percent of pulses, so most of the precious microcrystals end up unused in the collection container," says DESY scientist Alke


*"Our approach not only reduces the data collection time and the quantity of sample needed, it also opens up the opportunity of analysing entire viruses using X-ray lasers"*

*Alke Meents, DESY/CFEL*

Meents, who is based at the Center for Free-Electron Laser Science (CFEL) in Hamburg, a cooperation of DESY, the University of Hamburg and the German Max Planck Society. The standard methods therefore typically require several hours of beamtime and significant amounts of sample material in order to unravel the biomolecules' structure.

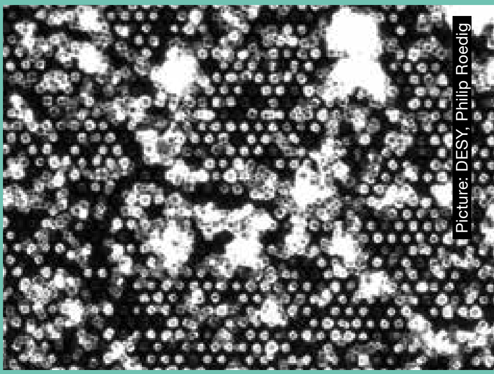
To use the limited beamtime and the precious sample material more efficiently, the team led by DESY physicist Meents developed a new method. The scientists use a micropatterned chip containing thousands of tiny pores to hold the protein crystals. The X-ray laser then scans the chip line by line, ideally allowing a diffraction image to be recorded for each pulse of the laser.

The researchers tested their method on two different virus samples using the LCLS X-ray laser at the SLAC National Accelerator Laboratory in the USA, which produces 120 pulses per second. They loaded their sample holder with a small amount of microcrystals of the bovine enterovirus 2 (BEV2), a virus that can cause miscarriages, stillbirths and infertility in cattle, and which is very difficult to crystallise. In this experiment, the scientists achieved a hit rate – where the X-ray laser successfully targeted the crystal – of up to nine percent. Within just 14 minutes, they had collected enough data to determine the correct structure of the virus – which was already known from experiments at other X-ray light sources – down to a scale of 0.23 nanometres (millionths of a millimetre).

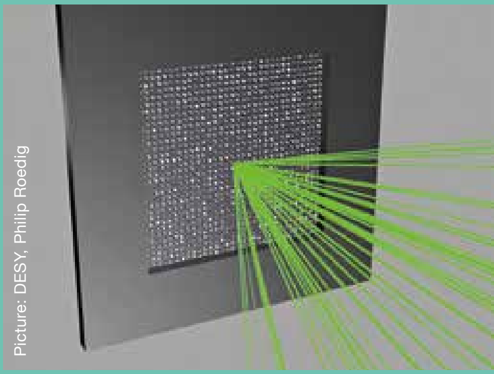
"To the best of our knowledge, this is the first time the atomic structure of an intact virus particle has been determined using an X-ray laser," Meents points out. "Whereas earlier methods at other X-ray light sources required crystals with a total volume of 3.5 nanolitres, we managed using crystals that were more than ten times smaller, having a total volume of just 228 picolitres."

This experiment was conducted at room temperature. While cooling the protein crystals – as is usually done in X-ray cristallography – would protect them to some extent from radiation damage, this is not generally feasible when working with extremely sensitive virus crystals. Crystals of isolated virus proteins are more robust, however, and can be frozen. In a second experiment, the researchers therefore studied the viral protein polyhedrin, which makes up a viral occlusion body for up to several thousands of virus particles of certain species. The virus particles use these containers to protect themselves against environmental influences and are thus able to remain intact for much longer times even under the most adverse conditions.

The scientist loaded their chip with polyhedrin crystals and examined them using the X-ray laser while keeping the chip ››




Micrograph of the microstructured chip, loaded with crystals for the investigation. Each square is a tiny crystal.




Schematic of the experimental setup: The chip loaded with nanocrystals is scanned by the X-ray beam (green) pore by pore. Ideally, each crystal produces a distinctive diffraction pattern.

at temperatures below minus 180 degrees Celsius. This time, the scientists achieved a hit rate of up to 90 percent. In just ten minutes, they had recorded more than enough diffraction images to determine the protein structure to within 0.24 nanometres. “For the structure of polyhedrin, we only had to scan a single chip, which was loaded with four micrograms of protein crystals; that is orders of magnitude less than the amount that would normally be needed,” explains Meents.

“Our approach not only reduces the data collection time and the quantity of sample needed, it also opens up the opportunity of analysing entire viruses using X-ray lasers,” Meents sums up. The scientists now want to increase the capacity of their chip by a factor of nearly ten, from 22 500 to some 200 000 micropores, and to further increase the scanning speed to up to one thousand samples per second. This would enable researchers to better exploit the potential of the new European XFEL X-ray free-electron laser, which has just started up in the Hamburg region and which will be able to produce up to 27 000 pulses per second. Furthermore, the next generation of chips will only expose the micropore that is being analysed, to prevent the remaining crystals from being damaged by scattered radiation from the X-ray laser.

*Nature Methods, 2017;*
*DOI: 10.1038/nmeth.4335*

# Transparent ceramics make superhard windows

A Japanese–German team of researchers has synthesised the first transparent sample of a popular industrial ceramic at DESY. The result is a superhard window made of cubic silicon nitride that can potentially be used under extreme conditions like in engines. Cubic silicon nitride forms under high pressure and is the second-hardest transparent nanoceramic after diamond but can withstand substantially higher temperatures.

“Silicon nitride is a very popular ceramic in industry,” explains research leader Norimasa Nishiyama from DESY, who now is an associate professor at Tokyo Institute of Technology. “It is mainly used for ball bearings, cutting tools and engine parts in the automotive and aircraft industry.” The ceramic is extremely stable, because the silicon–nitrogen bond is very strong. At ambient pressures, silicon nitride has a hexagonal crystal structure, and sintered ceramic of this phase is opaque. Sintering is the process of forming macroscopic structures from grain material using heat and pressure. The technique is widely used in industry for a broad range of products from ceramic bearings to artificial teeth.

At pressures above 13 gigapascals (GPa) – that is, 130 000 times the atmospheric pressure – silicon nitride transforms into a crystal structure with cubic symmetry. “The cubic phase of silicon nitride was first synthesised by a research group at Technical University of Darmstadt in 1999, but knowledge of this material is very limited,” says Nishiyama. His team used a large-volume press (LVP) at DESY to expose hexagonal silicon nitride to high pressures and temperatures. At 15.6 gigapascals – that is, approximately 156 000 times the atmospheric pressure – and a temperature of 1800 degrees Celsius, a transparent piece of cubic silicon nitride formed, with a diameter of about two millimetres. “It is the first transparent sample of this material,” emphasises Nishiyama.

Analysis of the crystal structure at DESY’s X-ray light source PETRA III showed that the initially hexagonal silicon nitride had completely transformed into the cubic phase. “The transformation is similar to carbon, which also has a hexagonal crystal structure at ambient conditions and transforms into a transparent cubic phase called diamond at high pressures,” explains Nishiyama. “However, the transparency of silicon nitride strongly depends on the grain boundaries. The opaqueness arises from gaps and pores between the grains.”

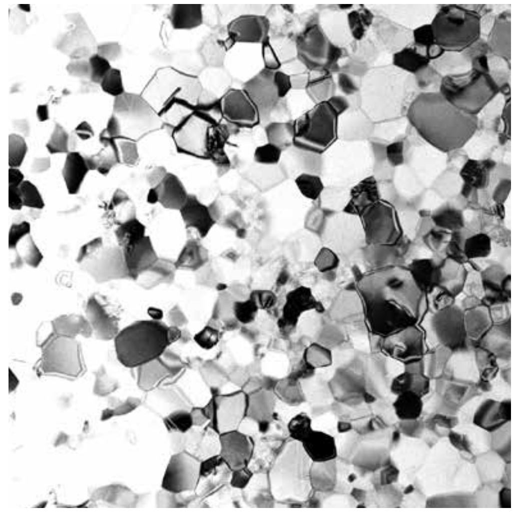
Investigations with a scanning transmission electron microscope at the University of Tokyo showed that the high-pressure sample has only very thin grain boundaries. “Also, in the high-pressure phase, oxygen impurities are distributed throughout the material and do not accumulate at the grain boundaries like in the low-pressure phase. That’s crucial for the transparency,” says Nishiyama. The scientists foresee diverse industrial applications for their superhard windows. “Cubic silicon nitride is the third-hardest ceramic known, after diamond and cubic boron nitride,” explains Nishiyama.

> *“Cubic silicon nitride is the third-hardest ceramic known, after diamond and cubic boron nitride”*
>
> *Norimasa Nishiyama, DESY/Tokyo Tech*

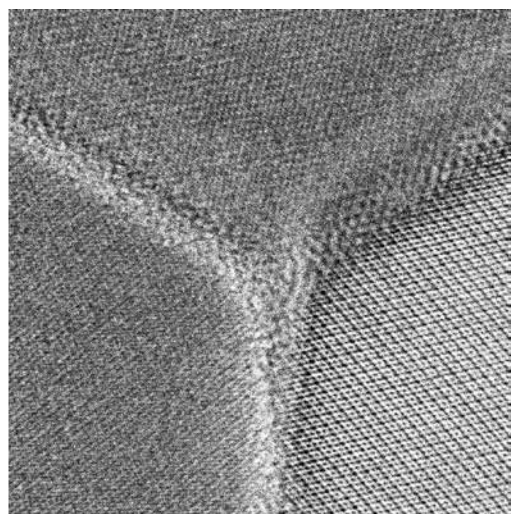
“But boron compounds are not transparent, and diamond is only stable up to approximately 750 degrees Celsius in air. Cubic silicon nitride is transparent and stable up to 1400 degrees Celsius.”

However, because of the large pressure needed to synthesise transparent cubic silicon nitride, the possible window size is limited for practical reasons. “The raw material is cheap, but to produce macroscopic transparent samples we need approximately twice the pressure as for artificial diamonds,” says Nishiyama. “It is relatively easy to make windows with diameters of one to five millimetres. But it will be hard to reach anything over one centimetre.”

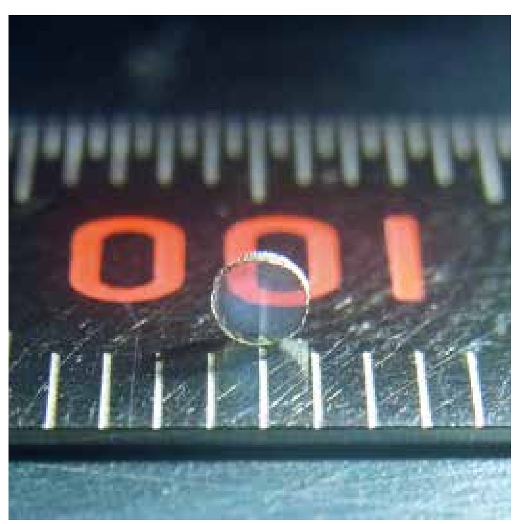
*Scientific Reports, 2017; DOI: 10.1038/srep44755*



Bright-field transmission electron microscope image of cubic silicon nitride. The average grain size is about 150 nanometres (millionths of a millimetre).



Atomic-resolution scanning transmission electron microscope image of a triple junction of grains in cubic silicon nitride. The thickness of the grain boundaries is less than one nanometre.




Approximately two-millimetre-large sample of transparent polycrystalline cubic silicon nitride, synthesised at DESY

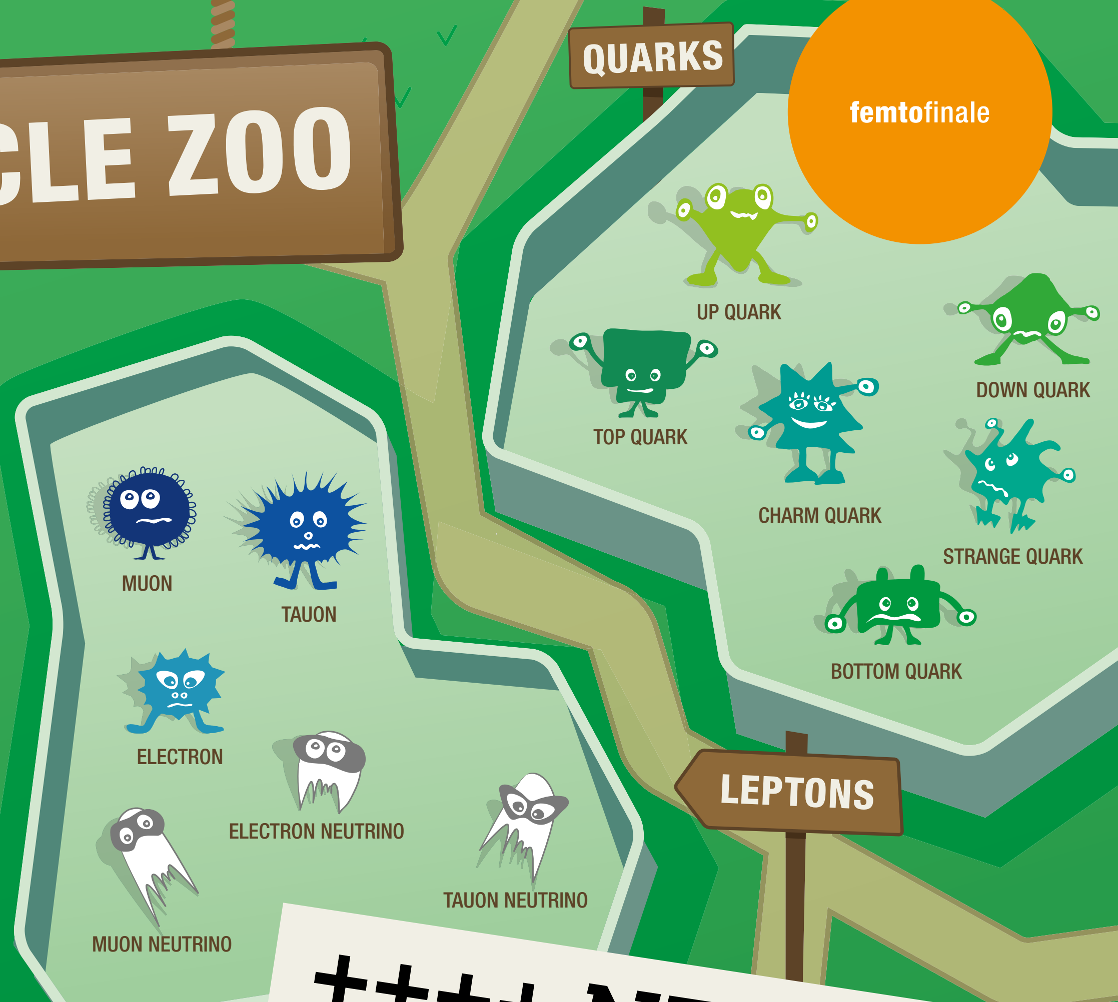
Pictures: DESY/Tokyo Tech, Norimasa Nishiyama

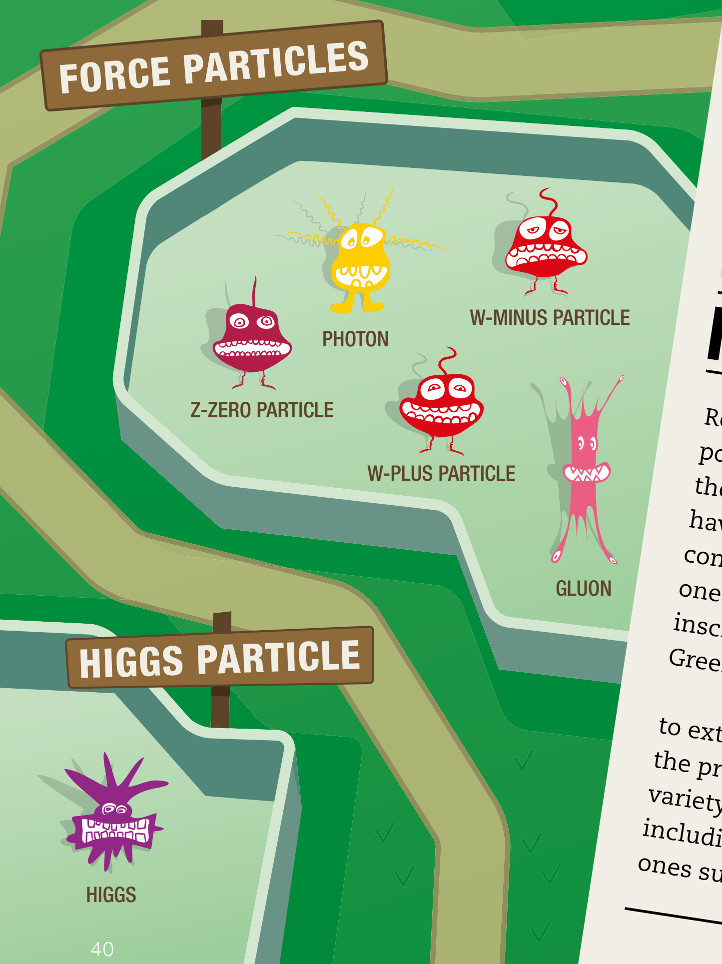
# PARTICLE ZOO

## WELCOME TO THE PARTICLE ZOO

Here you can see the smallest building blocks of the universe: particles that matter is made of, and force particles that mediate interactions between the matter particles.

We and everything around us are composed of three different types of particle: up quarks, down quarks and electrons. A major crowd-puller in this "zoo" is the Higgs particle, which was discovered at the LHC in 2012 and gives the other particles their mass.




## ++++ NEWS ++++

## NEW PARTICLE DISCOVERED!

Researchers at the world's most powerful particle accelerator, the Large Hadron Collider (LHC), have discovered a new particle. It consists of two charm quarks and one up quark and has the rather inscrutable name of $\Xi_{cc}^{++}$ ($\Xi$ is the Greek letter Xi).

The LHC accelerates protons to extremely high energies. When the protons collide, they create a variety of wildly different particles, including previously unknown ones such as the $\Xi_{cc}^{++}$, which, however, decays after only a fraction of a second. The newly discovered particle is the first one consisting of two heavy quarks and one light quark. "It doesn't play a role in our daily lives," explains DESY researcher Wilfried Buchmüller, who teaches theoretical elementary particle physics at the University of Hamburg. "It is another part of the puzzle that enables us to improve the previous models and theories of particle physics."

# Imprint

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**Editorial board address**
Notkestraße 85, 22607 Hamburg, Germany
Tel.: +49 40 8998-3613, fax: +49 40 8998-4307
e-mail: femto@desy.de
Internet: www.desy.de/femto
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**Editorial board**
Till Mundzeck (responsible under press law),
Ute Wilhelmsen

**Contributors to this issue**
Nikolai Promies

**Design and production**
gutentag Hamburg

**Translation**
TransForm, Cologne
Ilka Flegel, Kapellendorf

**Printing and image processing**
EHS, Hamburg

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## The DESY research centre

DESY is one of the world's leading particle accelerator centres. Researchers use the large-scale facilities at DESY to explore the microcosm in all its variety – ranging from the interaction of tiny elementary particles to the behaviour of innovative nanomaterials and the vital processes that take place between biomolecules. The accelerators and detectors that DESY develops and builds at its locations in Hamburg and Zeuthen are unique research tools. The DESY facilities generate the most intense X-ray radiation in the world, accelerate particles to record energies and open up completely new windows onto the universe.

DESY is a member of the Helmholtz Association, Germany's largest scientific organisation.

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES