

# femto

The DESY research magazine – Issue 02/20

ZOOM

## The strangest liquid in the world

Water amazes scientists  
time and again

Coronavirus proteins  
in X-ray vision

Plastic from wood

Spraying nanopaper



### Scientists film ultrafast molecular rotation

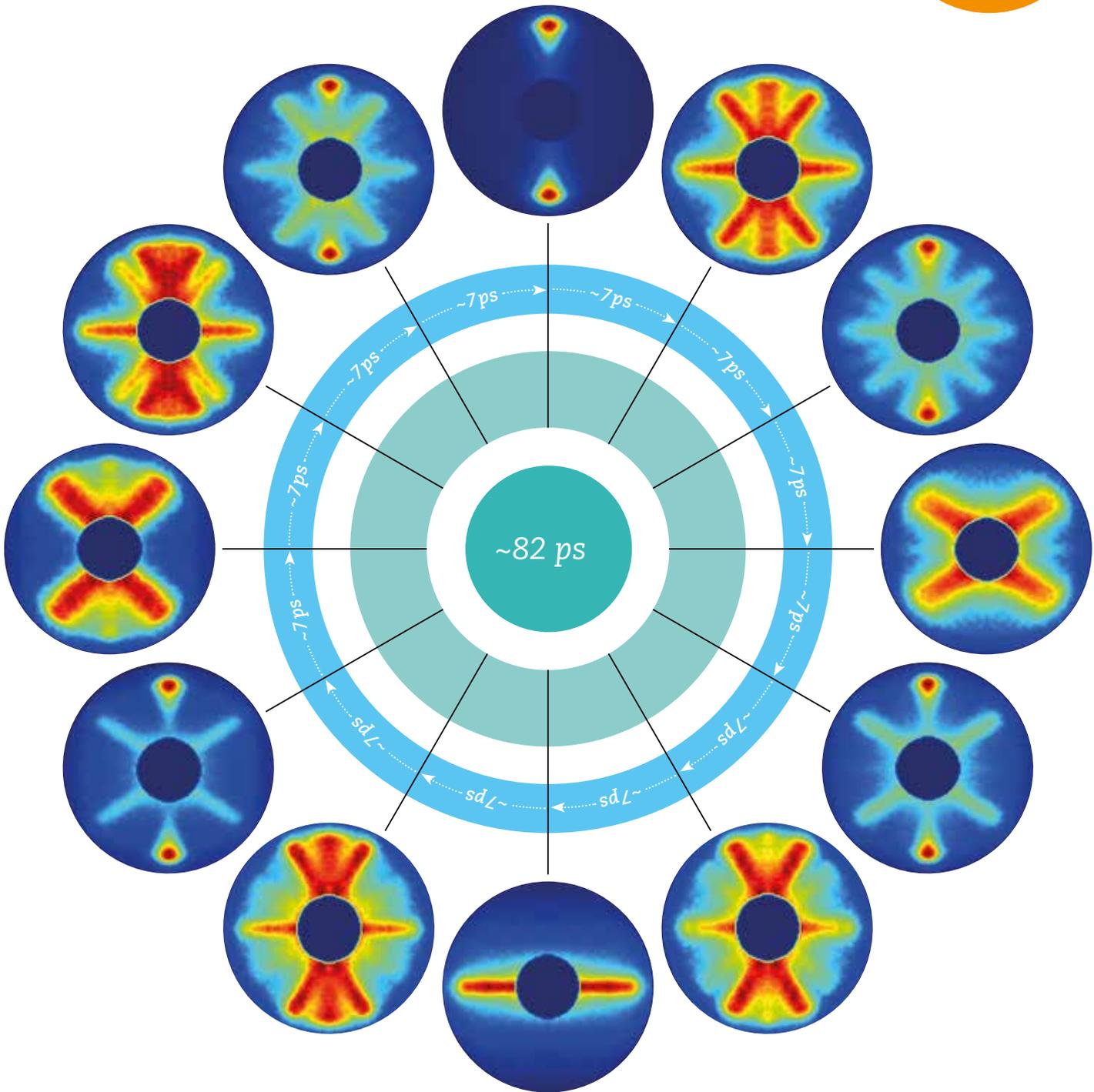
Scientists have used precisely tuned pulses of laser light to film the ultrafast rotation of a molecule. The resulting “molecular movie” tracks one and a half revolutions of carbonyl sulphide – a rod-shaped molecule consisting of one oxygen, one carbon and one sulphur atom – taking place within 125 trillionths of a second, at high temporal and spatial resolution.

“Molecular physics has long dreamed of capturing the ultrafast motion of atoms during dynamic processes on film,” explains DESY scientist Jochen Küpper from the Center for Free-Electron Laser Science (CFEL). To achieve this, Küpper’s team used two pulses of infrared laser light, which were precisely tuned to each other and separated by 38 trillionths of a second (picoseconds), to set the carbonyl sulphide molecules spinning rapidly in unison (i.e. coherently). They then used a further laser pulse with a longer wavelength to determine the position of the molecules at intervals of around 0.2 trillionths of a second each.

Altogether, the scientists took 651 pictures covering one and a half periods of rotation of the molecule. Assembled sequentially, the pictures produced a 125-picosecond-long movie of the molecule’s rotation.

“It would be wrong to think of the molecule’s motion as being like that of a rotating stick, though,” says Küpper. “The processes we are observing here are governed by quantum mechanics. On this scale, very small objects like atoms and molecules behave differently from the everyday objects in our surroundings. The position and momentum of a molecule cannot be determined simultaneously with the highest precision; you can only define a certain probability of finding the molecule in a specific place at a particular point in time.”

The scientists believe that their method can also be used for other molecules and processes in order to produce detailed movies of their dynamics.



Steps of the molecule's rotation, recorded at an average interval of seven picoseconds

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Picture: Victor Serban, Unsplash

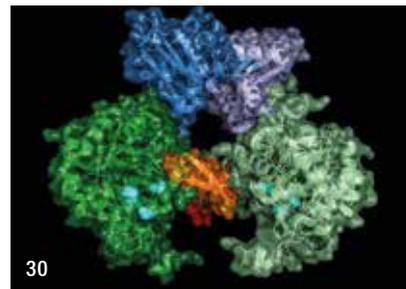
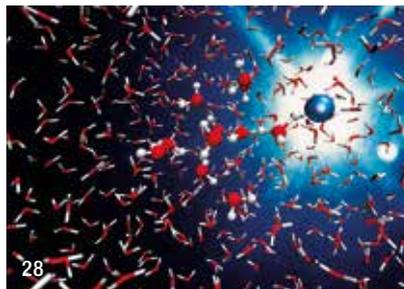
## ZOOM

# The strangest liquid in the world

**Water is commonplace – but still not fully understood by science**

Water is everywhere – and at the same time one of the most astonishing chemical compounds. It expands when you cool it down, and under certain circumstances it freezes when you heat it up. It is virtually incompressible, has an unusually high heat capacity, and its high surface tension enables it to creep up walls.

Water is the element of life – many of its surprising properties are essential for life as we know it. Despite centuries of research, the relatively simple molecule continues to astonish scientists. “Of all known liquids, water is probably the most studied and least understood,” according to British chemist Felix Franks, a pioneer of water research. Now, the interdisciplinary Centre for Molecular Water Science (CMWS) at DESY is to advance research into the world’s most unusual liquid.



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# Coronavirus proteins in X-ray vision

## Screening identifies potential drug candidates

**C**an the new coronavirus be stopped with drugs? Research groups around the world are intensively searching for starting points for an active ingredient against SARS-CoV-2, as the virus was named by the World Health Organization (WHO). Like many centres worldwide, DESY is also participating in the fight against the pandemic. Various teams are searching for new active ingredients, investigating the molecular biological processes of the infection or X-raying damaged tissue in 3D. Research topics further include possible rapid tests, innovative ways of accurately dosing possible corona drugs and the evaluation of data from a corona app using big-data methods from particle physics. In addition, the DESY workshops have started the production of face shields, which are made available to physicians and nursing homes.

### Rapid access

For research projects related to the new coronavirus, DESY offers, among other things, rapid access to its X-ray light source PETRA III, which remained open for corresponding projects even during the period of temporarily reduced operation of the DESY facilities. For example, with the help of PETRA III, a research team has already identified several candidates for possible active ingredients that bind to an important protein of the SARS-

CoV-2 pathogen and that could thus be a basis for a drug against the infection.

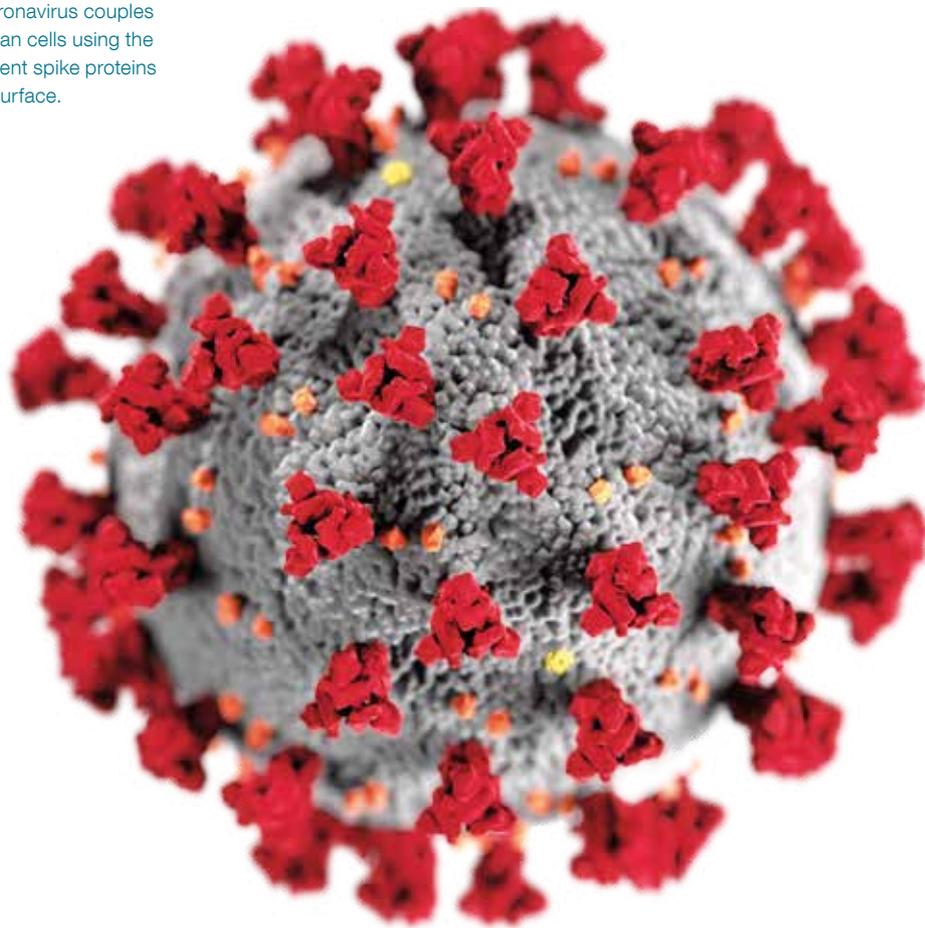
### High-throughput procedure

For this study, the researchers first grow small crystals of the viral protein in combination with a potential active ingredient. They then investigate these crystals using X-rays to determine their detailed atomic structure and thus find out whether and where the active ingredient binds to the viral protein. In a high-

throughput procedure, the team uses this method to test almost 6000 known active ingredients from a library at the Fraunhofer Institute for Molecular Biology and Applied Ecology. Thanks to a fully automatic sample change with a robotic arm, each measurement takes only three minutes.

After measuring 7697 samples containing 4035 different active ingredients, the scientists have already been able to identify 18 substances that bind to the main protease (MPro) of the pathogen –

The coronavirus couples to human cells using the prominent spike proteins on its surface.



a key protein for the replication of the virus in the human body. Whether these substances inhibit protein activity and slow down the replication of the virus, however, will only be revealed in further laboratory tests.

### Promising starting points

Proteins that play a key role for the multiplication of the virus are promising starting points for

study have already been approved for the treatment of humans or are at least in the trial stage.

“With the help of automated data analysis, after only two weeks we were already able to identify more than a dozen active substances that bind to the proteins,” says DESY scientist Alke Meents, who leads the study. “One of them binds covalently, that is with a very strong chemical bond,

*“After only two weeks, we were already able to identify more than a dozen active substances that bind to the proteins”*

Alke Meents, DESY

antiviral drugs. Viruses cannot replicate on their own. To do so, they hijack cells of their host, introduce their own genetic material into the cells and induce them to produce new viruses. Proteins play an important role in all these steps. If one of these key proteins can be blocked, it may be possible to stop the replication of the virus and thus defeat the infection.

Several measuring stations at DESY’s light source PETRA III specialise in structural biological investigations. Here, the three-dimensional spatial structure of proteins can be resolved with atomic precision. The research team used these capabilities to examine several thousand active ingredients already in existence for the treatment of other diseases in order to find out whether and how they “dock” to one of the key proteins responsible for the replication of the virus. With this investigation, the team hopes to shorten the path to a drug: While the development of an approved drug from a new compound usually takes several years, some of the substances investigated in this

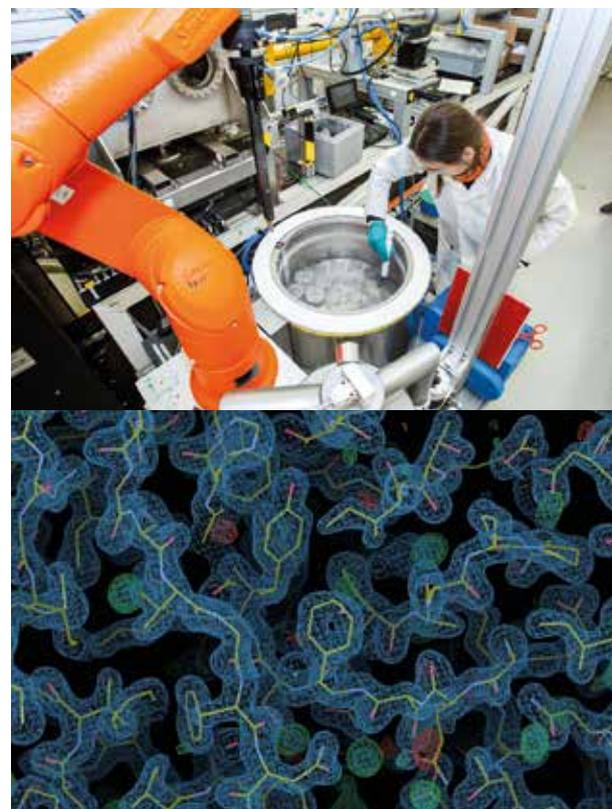
at a central location to the main protease of the virus, making it a particularly promising candidate.”

### The long way to a drug

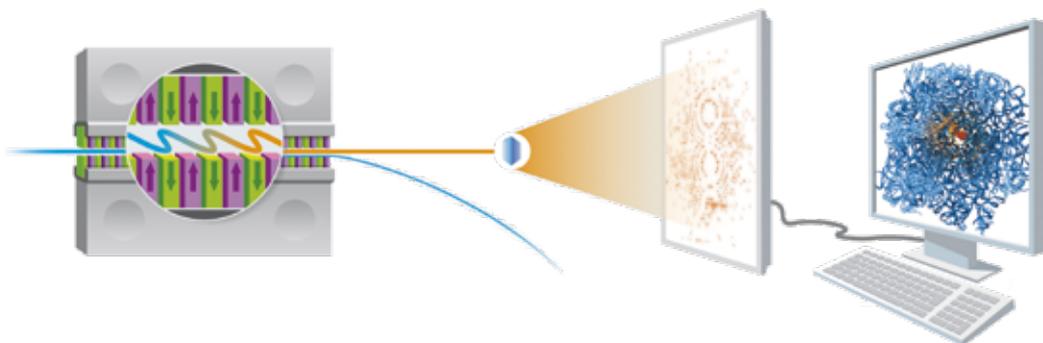
However, the identification of promising substances is only the first step on the way to a drug. “Researchers at the universities of Lübeck and Hamburg and from the Fraunhofer Institute are investigating in the laboratory whether this active substance also inhibits protein activity,” says virus researcher Rolf Hilgenfeld from the University of Lübeck, whose

group is involved in the screening. In a third step, the Bernhard Nocht Institute for Tropical Medicine in Hamburg is testing in cell cultures whether the substance inhibits or even prevents virus replication. However, even then the road to an approved drug is still long.

The samples are cooled in a tank with liquid nitrogen and automatically positioned in the X-ray beam by a robot arm.



Section of the electron density map of the SARS-CoV-2 main protease



### Structural analysis of biomolecules with X-rays

Fast electrons (blue) from a particle accelerator are sent into an undulator (left) equipped with powerful magnets (green and violet). The electrons race past the magnets in a slalom pattern. In the process, the particles emit high-energy X-ray radiation (orange), which is directed through X-ray optics at a crystal (centre) made up of biomolecules. The crystal diffracts the X-rays, thus generating a characteristic diffraction pattern on the detector (right). From this diffraction pattern, the structure of the biomolecules under investigation can be calculated down to the last atom (far right).

Gamma-ray bursts can be triggered by the explosion of a dying, supermassive star collapsing into a black hole. From the vicinity of the black hole, powerful jets of matter shoot in opposite directions into space, accelerating electrically charged particles, which in turn interact with magnetic fields and radiation to produce gamma rays.

# Cosmic gamma-ray bursts with record energy

First detection with ground-based gamma-ray telescopes

**T**he strongest explosions in the universe produce even more energetic radiation than previously known: Using specialised telescopes, two international teams of researchers have registered the highest-energy gamma rays ever measured from so-called gamma-ray bursts, reaching energies that are about 100 billion times higher than that of visible light. The scientists of the H.E.S.S. and MAGIC telescopes presented their observations in independent publications in the journal *Nature*. These are the first detections of gamma-ray bursts with ground-based gamma-ray telescopes. DESY plays a major role in both observatories, which are operated under the leadership of the Max Planck Society.

## Explosion of giant suns

Gamma-ray bursts (GRBs) are sudden, short bursts of gamma radiation happening about once a day somewhere in the visible universe. According to current knowledge, the gamma-ray flashes originate from colliding neutron stars or from supernova explosions of giant suns collapsing into a black hole. "Gamma-ray bursts are the most powerful explosions known in the universe and typically release more energy in just a few seconds than our sun during its entire

*"These are by far the highest-energy photons ever discovered from a gamma-ray burst"*

Elisa Bernardini, DESY

lifetime – they can shine through almost the entire visible universe," explains David Berge, head of gamma-ray astronomy at DESY.

## Two international teams

The cosmic phenomenon was discovered by chance at the end of the 1960s by satellites used to monitor compliance with the nuclear test ban on Earth. Since then, astronomers have been studying gamma-ray bursts with satellites from Earth orbit, as the Earth's atmosphere very effectively absorbs gamma rays, preventing ground-based telescopes from detecting them.

Astronomers have developed specialised telescopes that can observe a faint blue glow called Cherenkov light that cosmic gamma rays induce in the Earth's

*“Gamma-ray bursts are the most powerful explosions known in the universe and typically release more energy in just a few seconds than our sun during its entire lifetime”*

David Berge, DESY

of the US space agency NASA that monitor the sky for gamma-ray bursts and send automatic alerts to other gamma-ray observatories, such as H.E.S.S. and MAGIC, upon detection. “We were able to point to the region of origin so quickly that we could start observing only 57 seconds after the initial detection of the explosion,” reports DESY researcher Cosimo Nigro from the MAGIC group at DESY, who was in charge of the observation shift at that time. “In the first 20 minutes of observation, we detected about thousand photons from GRB 190114C.”

#### More than four billion light years

MAGIC registered gamma rays with energies between 200 and 1000 billion electronvolts (0.2 to 1 teraelectronvolts). “These are by far the highest-energy photons ever discovered from a gamma-ray burst,” says Elisa Bernardini, leader of the MAGIC group at DESY. For comparison: Visible light lies in the energy range of about 1 to 3 electronvolts.

The rapid discovery made it possible to quickly alert the entire observational community. As a result, more than 20 different telescopes took a closer look at the target in various wavelength ranges. In this way, details of the physical mechanisms responsible for the highest-energy emission could be deciphered. Follow-up observations placed GRB 190114C at a distance of more than four billion light years. This means that its light travelled more than four billion years to us, or about a third of the current age of the universe.

At a distance of six billion light years, GRB 180720B was even further away. Nonetheless, its gamma-ray emission at energies between 100 and 440 billion electronvolts could still be detected long after the initial blast.

The detection of gamma-ray bursts at very high energies provides important new insights into the gigantic explosions. “Having established that GRBs produce photons of energies hundreds of billion times higher than visible light, we now know that GRBs are able to efficiently accelerate particles within the explosion ejecta,” says DESY researcher Konstancja Satalecka, one of the scientists coordinating GRB searches in the MAGIC collaboration. “What’s more, it turns out we were missing approximately half of their energy budget until now. Our measurements show that the energy released in very-high-energy gamma rays is comparable to the amount radiated at all lower energies taken together. That is remarkable!”

*Nature, 2019; DOI: 10.1038/s41586-019-1743-9*

*Nature, 2019; DOI: 10.1038/s41586-019-1750-x*

*Nature, 2019; DOI: 10.1038/s41586-019-1754-6*

atmosphere. For many years, scientists had been trying to catch a gamma-ray burst with such Cherenkov telescopes. Then, between summer 2018 and January 2019, two international teams of astronomers, both involving DESY scientists, detected gamma rays from two GRB events for the first time from the ground.

On 20 July 2018, faint afterglow emission of GRB 180720B in the gamma-ray regime was observed with the 28-metre telescope of the High-Energy Stereoscopic System (H.E.S.S.) in Namibia. On 14 January 2019, bright early emission from GRB 190114C was detected by the Major Atmospheric Gamma Imaging Cherenkov (MAGIC) telescopes on La Palma.

Both observations were triggered by gamma-ray satellites

# Plastic from wood

## Lignin-based components made to measure

The biopolymer lignin is a by-product of paper making and a promising raw material for manufacturing sustainable plastic materials. However, the quality of this naturally occurring product is not as uniform as that of petroleum-based plastics. An X-ray analysis carried out at DESY reveals for the first time how the internal molecular structure

compounds, which also play a key role in manufacturing synthetic polymers or plastics. “Lignin is the biggest source of naturally occurring aromatic compounds, but until now it has been viewed by the paper industry primarily as a by-product or a fuel,” explains Mats Johansson from the Royal Institute of Technology (KTH) in Stockholm, who led the research

of commercially available lignin at DESY’s X-ray source PETRA III. “It turns out that there are lignin fractions with larger and smaller domains,” reports the main author Marcus Jawerth of KTH Stockholm. “This can offer certain advantages, depending on the particular application: It makes the lignin harder or softer by altering the so-called glass transition temperature at which the biopolymer adopts a viscous state.”

### Numerous configurations

Among other things, the X-ray analysis revealed that those types of lignin whose central benzene rings are arranged in the shape of a T are particularly stable. “The molecular structure affects the macroscopic mechanical properties,” explains DESY researcher Stephan Roth. “This is the first time this has been characterised.” As a natural product, lignin comes in numerous different configurations. Further studies are needed to provide a systematic overview of how different parameters affect the properties of the lignin. “This is very important in order to be able to manufacture materials reproducibly and in particular to predict their properties,” says Roth, who is also a professor at KTH Stockholm. “If you want to use a material industrially, you need to understand its molecular structure and know how this is correlated with the mechanical properties.”

According to Jawerth, up to two thirds of the lignin produced during paper making could be turned into polyesters and serve as a starting material for making plastics. “Along with cellulose and chitin, lignin is one of the most ubiquitous organic compounds on Earth and offers enormous potential for replacing petroleum-based plastics,” says the scientist. “It’s far too valuable to simply burn it.”

*“Along with cellulose and chitin, lignin is one of the most ubiquitous organic compounds on Earth and offers enormous potential for replacing petroleum-based plastics. It’s far too valuable to simply burn it.”*

Marcus Jawerth, KTH Stockholm

of different lignin fractions is related to the material properties. The study provides an approach for a systematic understanding of lignin as a raw material for producing bioplastics with different properties, depending on the specific application.

Lignin is responsible for the stability of plants, stiffening them and making them “woody”. During paper production, lignin is separated from cellulose. Lignin forms so-called aromatic

team. “Millions of tonnes of it are produced every year, providing a steady stream of raw material for new potential products.”

### Nanostructure

Some first applications of hard lignin-based plastics (thermosets) already exist. However, their material properties often vary, and it has been difficult to control them specifically. The Swedish team has now shed light on the nanostructure of different fractions

Lignin is a group of macromolecules that are embedded in the plant cell wall and cause lignification.

Marcus Jawerth graduated on lignin-based plastics at KTH Stockholm.



Applied Polymer Materials, 2020;  
DOI: 10.1021/acsapm.9b01007



The larva fossil in amber. Its age is between 42 and 49 million years, at most 54 million years. It was examined at the Institute of Zoology and Evolutionary Research at the University of Jena.

# Ancient parasite in amber

Research team unravels secrets of 50-million-year-old parasite larva

Using the intense X-ray radiation from DESY's particle accelerator PETRA III, researchers have investigated an unusual find: a 50-million-year-old insect larva from the era of the Palaeogene. The results offer a unique insight into the development of the extinct insect.

## A find on eBay

When the biologist Hans Pohl from the Friedrich Schiller University in Jena tracked down an insect fossil trapped in amber on eBay, the joy of discovery was great: It was a special specimen, a 50-million-year-old larva of an extinct twisted-wing insect from the order of *Strepsiptera*. But in order to be able to investigate it in detail, he needed the help of materials researchers from the Helmholtz Centre Geesthacht (HZG), which operates a beamline at DESY's X-ray source PETRA III.

*Strepsiptera* are parasites that infest other insects, such as bees and wasps, but also silverfish. "In most of the approximately 600 known species, the females remain in their host throughout

their lives," says Pohl. "Only the males leave it for the wedding flight, but then live only a few hours." But there are exceptions: In species that infest silverfish, the wingless females also leave their host.

## 3D X-ray images

The 4.4-millimetre-long animal was enclosed and sealed by tree resin approximately 50 million years ago. It is the first known larva fossil of a twisted-wing insect that has developed past the first larval stage.

The problem: "Under the light microscope, essential details could not be seen," explains Pohl. His team therefore opted to investigate the fossil using a high-resolution X-ray method – microtomography with synchrotron radiation.



Model of the larva in the amber generated from the X-ray images

The PETRA III storage ring is particularly well suited for this purpose. Here, the Helmholtz Centre Geesthacht (HZG) operates a measuring station that usually deals with materials research. "The method is similar to a CT scanner in a hospital, producing three-dimensional X-ray images of the inside of a body," says HZG researcher Jörg Hammel.

The method delivered pin-sharp images of the twisted-wing larva with a resolution of 1.3 micrometers. "All its important details can be seen," Hans Pohl says. "Among other things, we were able to observe that it was probably in its third larval stage and that it was very likely a female larva of *Mengea*, a genus that is extinct today." What is special is that the female larva had left its host – a behaviour known only from the silverfish parasites among today's *Strepsiptera* species. "Some evidence suggests that the host may have been a cockroach," reports Pohl. "To be certain, however, we would have to track down and analyse more fossils."

It is quite possible that these analyses will then again be conducted at PETRA III. "In recent years, the HZG beamline seems to have become an insider tip among biologists," says Jörg Hammel. "Apparently, we have become so good at analysing amber fossils that we are receiving more and more enquiries from experts."

*Arthropod Systematics & Phylogeny*, 2019;  
DOI: 10.26049/ASP77-1-2019-06

ZOOM

# The strangest liquid in the world

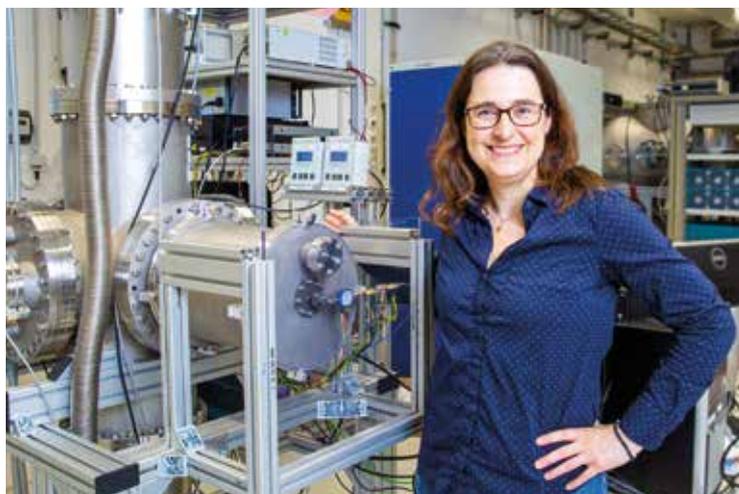
**Water is commonplace – but still  
not fully understood by science**

Water is everywhere – and at the same time one of the most astonishing chemical compounds. It expands when you cool it down, and under certain circumstances it freezes when you heat it up. It is virtually incompressible, has an unusually high heat capacity, and its high surface tension enables it to creep up walls. Water is the element of life – many of its surprising properties are essential for life as we know it. Despite centuries of research, the relatively simple molecule continues to astonish scientists. “Of all known liquids, water is probably the most studied and least understood,” according to British chemist Felix Franks, a pioneer of water research. Now, the interdisciplinary Centre for Molecular Water Science (CMWS) at DESY is to advance research into the world’s most unusual liquid.



Water forms an unusually large number of different kinds of ice, some having exotic properties. There are more than 20 types of frozen water, including a black high-pressure ice that would even remain stable at the temperatures found on the surface of the sun. The melting point of water is unexpectedly high too: about 100 degrees above that of similar compounds.

**S**treams babble, waves roar, rain patters, and the bathroom tap drips. Water is a faithful companion – as a grand spectacle of nature, as the basis of all life or simply as a damp nuisance. In the eyes of science, however, H<sub>2</sub>O remains a mystery. Although it consists of only three atoms – two hydrogens and one oxygen – this simple constellation leads to some remarkable properties. Instead of whizzing around as a gas at room temperature, like other comparable substances, water remains liquid in drinking cups and vases. Instead of becoming more and more viscous under increasing pressure, water becomes increasingly runny. And instead of sinking to the bottom, icebergs float majestically across the polar seas.



DESY's leading scientists Melanie Schnell and Gerhard Grübel are coordinating the Centre for Molecular Water Science (CMWS).



One of the anomalies of water is its exceptionally high surface tension, which allows it to form droplets.

Scientists are now aware of more than 50 such anomalies of water, without which we would not be here. “If water wasn’t so strange, we wouldn’t exist,” says Anders Nilsson from the University of Stockholm, one of the world’s most renowned water researchers. If water had the properties of a typical liquid, Hamburg’s climate would resemble that of deepest Siberia. And without the capillary action of water, plants would be unable to supply themselves with nutrients.

Very few of these anomalies are fully understood – a great deal of fundamental research is still needed to unravel the properties and interactions of the ubiquitous water molecules. Now, a new centre unlike any other in the world is to focus this research. Together with partners from all over Europe, DESY plans to set up the Centre for Molecular Water Science, or CMWS for short. The CMWS will be entirely

*“If water wasn’t so strange, we wouldn’t exist”*

Anders Nilsson, University of Stockholm

interdisciplinary and is to examine the subject of water from a wide range of different angles.

Physicists would like to study H<sub>2</sub>O under extreme conditions, for example, to uncover the molecular causes of its special properties. Biophysicists want to take a closer look at it in order to get to the bottom of the role it plays in cell metabolism, which has long been underrated. Climate researchers are interested

in knowing how tiny water droplets form in the atmosphere and pile up to form towering clouds – these are key players in global warming. And astrochemists are wondering how water in space can serve as a frosty breeding ground for all manner of compounds – including relatively complex organic molecules such as the precursors of amino acids, which may have given rise to life.

## “Supercooled water is a reality in nature”

Austen Angell, Arizona State University

The anomalies are most pronounced when water is supercooled. Contrary to our everyday experience, H<sub>2</sub>O does not necessarily crystallise to become ice at zero degrees Celsius. Especially when it is extremely pure, it can remain liquid down to very low temperatures, because there are no nuclei on which ice crystals can form.

“In clouds, the droplets can get as cold as minus 30 degrees Celsius,” says Austen Angell, a chemist at Arizona State University, who is a water specialist like Nilsson. “So, supercooled water is a reality in nature.”

### Water is unusual

Ice-cold water sometimes behaves in very unusual ways in the laboratory. In contrast to other materials, the colder it is, the easier it becomes to compress. A similar phenomenon can be observed with its heat capacity: The colder water becomes, the more heat it is able to absorb. Experts attribute these anomalies to the structure of the water molecule: The oxygen atom forms the “body”, with two hydrogen atoms branching off as “arms”. The body is slightly negatively charged, while the arms are positively charged. This causes water molecules to be attracted to each other: The negative body of one molecule is attracted towards the positive arms of another molecule – joining them briefly in the form of a hydrogen bond.

In that sense, water can be viewed as a billowing network of molecules. These are constantly forging spontaneous bonds with their neighbours – only to cut these delicate ties again

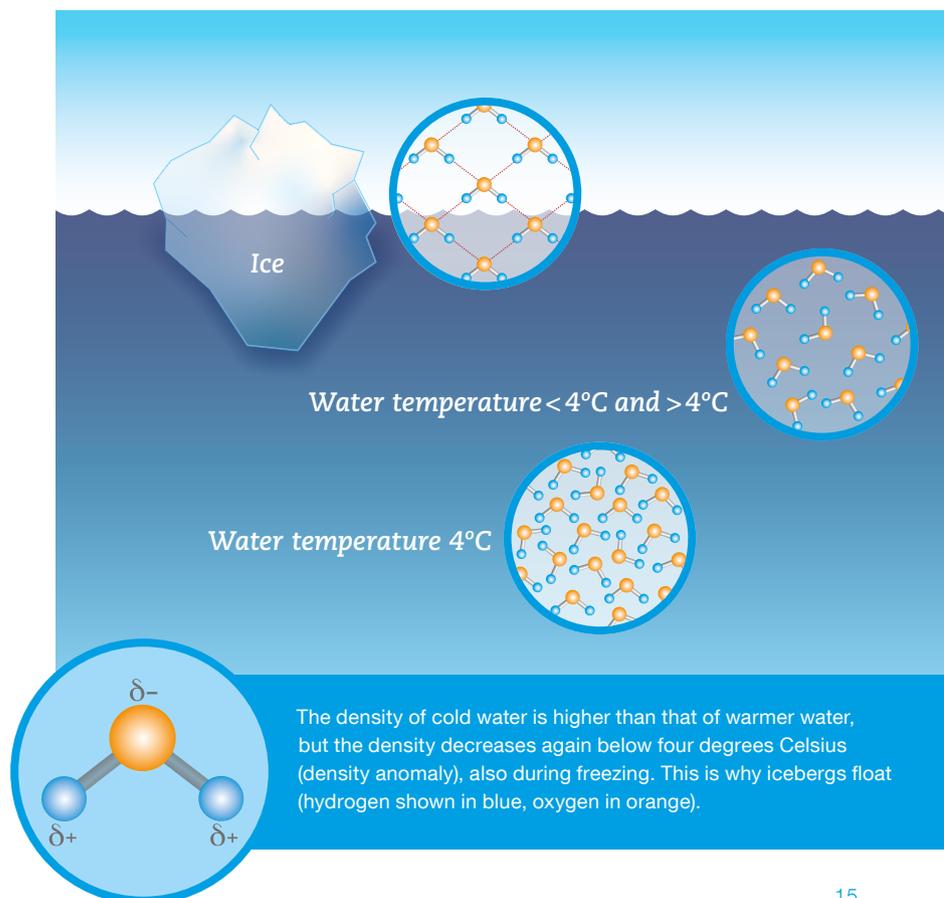
immediately. Experts have long suspected that water exists in two different states, depending on the number and orientation of the hydrogen bonds: a denser state (HDL = high-density liquid) and a less dense state (LDL = low-density liquid). The density of HDL is 10 to 20 percent higher than that of LDL. “Basically, water thus consists of two different types,” says Anders Nilsson.

“And we believe that the interplay between these two varieties is behind water’s anomalies.”

An ordinary glass of water at room temperature is likely to consist primarily of the HDL phase – with tiny clusters of 20 to 30 molecules briefly combining to form an LDL phase. “It’s as if the meatballs in your soup kept disappearing and reappearing again somewhere else,” Nilsson explains. The problem is that these balls are so short-lived that detecting them calls for new measuring techniques. The hope is that these techniques will make it possible to observe whether the miniature bubbles grow and become more stable at lower temperatures, thus proving the HDL/LDL hypothesis. >>



Austen Angell is one of the most renowned water researchers in the world.





When HDA ice is converted into LDA ice, the volume of ice spontaneously increases by about a quarter.

Two corresponding varieties have already been discovered in certain glass-like types of ice, i.e. the solid phase of water. They are called HDA (high-density amorphous) ice and LDA (low-density amorphous) ice – the density of the former being higher than that of the latter. In 2017, a team led by Anders Nilsson, DESY physicist Gerhard Grübel and Innsbruck ice researcher Thomas Lörting successfully performed a remarkable experiment in a ground-breaking collaboration. Using DESY's X-ray source PETRA III, the team was able to observe HDA ice melting to become HDL water when it was heated rapidly at minus 150 degrees Celsius. For the briefest moment, this mutated to become LDL water, only to turn into solid ice once again, but this time in the LDA form. The existence of two different types of water therefore seems to be confirmed at extremely low temperatures.

The specialists are now looking for final, conclusive proof – the detection of HDL and LDL in liquid water. Several teams are pursuing different strategies: In the USA, Austen Angell is focusing on adding specific salts to ultrapure water. “This allows us to lower the freezing point

without destroying the anomalous character of the water,” he explains – and hopes to find solid evidence of the existence of the two phases of water in the collected data.

### Water in the X-ray laser

Other teams are placing their hopes in a research tool that is still comparatively new – X-ray lasers such as the European XFEL. These generate ultrashort pulses of X-rays that can be used to analyse extremely rapid processes. “This allows us to cool water down extremely quickly and yet still observe what is happening to it,” explains Anders Nilsson, “because we capture the image even before the water can crystallise to become ice.”

One of the leading teams using X-ray lasers to explore this no-man's-land is headed by DESY scientist Gerhard Grübel. The centrepiece of his experiment, standing in the middle of his laboratory, is a metal structure consisting of two intersecting vacuum tubes, rather like the model of a space station. “We shoot a jet of extremely fine water droplets down one tube,” explains Grübel. “The ultrashort X-ray pulses, which we use to scan the droplets, are fired down the other.” The hope is that the droplets will be so



The European XFEL produces extremely bright, ultrashort X-ray laser pulses that can be used, among other things, to take snapshots of very rapid phenomena.

# CMWS Centre for Molecular Water Science

The CMWS is an international collaboration of experts in the field of water research.

More than 40 partners from universities and research institutions in Germany and abroad have got together and set up a joint research initiative to gain a fundamental understanding of the molecular processes that take place in water and at its boundary surfaces. The centre is thematically organised in five closely interlinked areas of research, which are working together to understand the role of water at the molecular level:



**Fundamental properties of water:**  
To what extent can its numerous anomalies be explained by the complex interplay between the H<sub>2</sub>O molecules?



**Water in climate, astro and Earth sciences:**  
What role does water play in the environment and the atmosphere?  
How does it behave in space and on far-off planets?



**Water in energy research and technology:**  
How can corrosion damage be minimised, catalytic reactions be accelerated and energy conversion be made more efficient?



**Chemical dynamics in real time:**  
What exactly happens when substances dissolve in water, when acids and bases attack, or when water is exposed to ionising radiation?



**Water in biochemical and biological processes:**  
How does H<sub>2</sub>O influence what happens in cells?  
What role does it play in cell transport and signalling?

Since 2019, in cooperation with DESY, an ongoing CMWS “Early Science” programme has been supporting research projects carried out by young scientists. An office has been set up to coordinate the initiative, and planning has begun for a research and laboratory building. Further information: [www.desy.de/cmws](http://www.desy.de/cmws)

highly supercooled that the coexistence of HDL and LDL should become clearly apparent.

To achieve this, the formation of the droplets needs to be extremely sophisticated. Water is squeezed into the vacuum tube through a micrometre-fine quartz nozzle. This creates very fine droplets that cool down so quickly that

*“The droplets literally explode when they are hit, and this can be observed on the images recorded by a high-speed camera”*

Gerhard Grübel, DESY

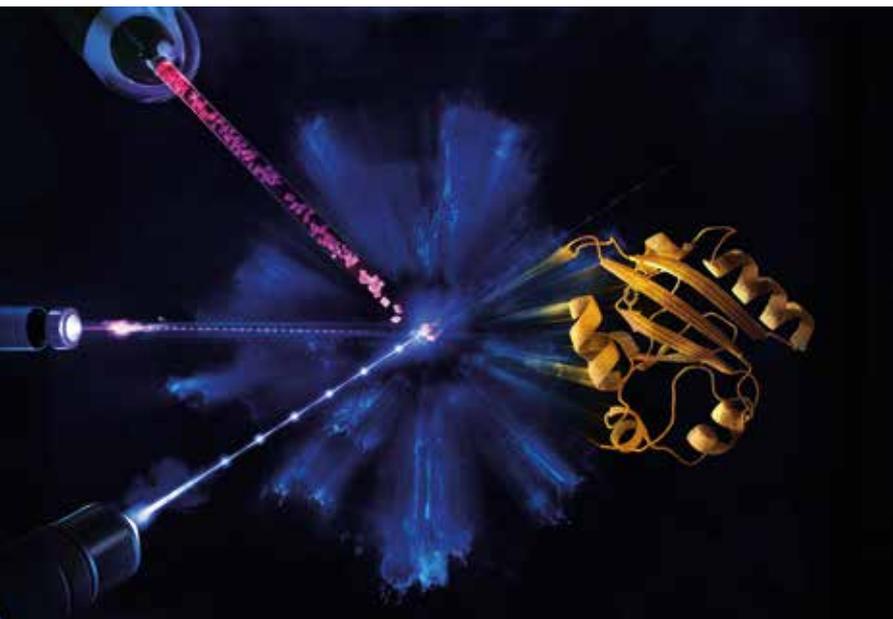
they have no time to crystallise. One behind the other, they shoot down the pipe towards the intersection.

“That’s where we have to get the droplets and X-ray pulses to collide,” explains Grübel, one

of DESY’s leading scientists and a coordinator of the water centre. The trick is to set up vibrations in the quartz nozzle with the help of a piezoelectric crystal, thereby controlling droplet formation, until the water and the X-rays collide. “It takes a bit of adjustment,” says Grübel. “The droplets literally explode when they are hit, and this can be observed on the images recorded by a high-speed camera.”

To carry out the experiments, the droplet gun is shipped to the most powerful X-ray lasers in the world, for example to Stanford in California. “The first experiments there were very promising,” says Grübel. “It looks as though structures made of dense and less dense water are actually showing up. However, they could also be precursors of ice.”

The scientists hope that experiments conducted at the European XFEL will provide further clues. “It can produce significantly more X-ray pulses per second than the Stanford machine, meaning that we can take many more pictures,” says Grübel. “Although there is a great deal of evidence suggesting that the model with the two phases of water is correct, we are still lacking direct verification.” >>



In serial femtosecond crystallography, a fine jet of water full of protein nanocrystals is fired across the path of an X-ray free-electron laser. When an X-ray pulse strikes a crystal, the latter immediately evaporates, but not before revealing information about its inner structure.

### Water is life

Crucially, however, H<sub>2</sub>O is essential for our existence – without water, there is no life. After all, about 50 to 65 percent of the adult human body consists of water. Among other things, water controls the fluid balance in the body, dissolves solid foods such as sugar, salt and vitamins and, as a coolant, protects the organism from overheating. It probably also

*“It may be a fundamental principle that certain protein reactions are regulated by such water networks”*

Henrike Müller-Werkmeister, University of Potsdam

plays a central role in the body’s cells. “However, we still know very little about what that water does and what functions it has,” says Henrike Müller-Werkmeister from the University of Potsdam. “We are only gradually starting to look into this.”

Among other things, H<sub>2</sub>O seems to be important in regulating the pH: Certain proteins can pump protons (hydrogen nuclei) into or out of cells. Short chains of water molecules probably serve as “climbing ropes” in this process. Water also seems to be closely involved when protein molecules are folded into their final shape after being assembled: Protein folding is much more sluggish if water

is replaced by its heavier cousin, known as heavy water.

Until now, however, methods for studying such processes in detail have been lacking. In protein crystallography, for example, in which powerful X-rays are used to unravel the structure of biomolecules right down to individual atoms, scientists usually work with frozen crystalline samples – these being better able to withstand the intense radiation. But as Müller-Werkmeister explains, “This doesn’t allow us to view the dynamic network of the water molecules in the proteins. The motion of the molecules is literally frozen.”

Now a new method, developed to a substantial degree in Hamburg, is providing a solution: time-resolved serial femtosecond crystallography. The idea is that the X-ray pulses no longer strike a relatively large, frozen protein crystal, but an extremely fine beam of many tiny crystals instead. Since each crystal only collides with an X-ray pulse once, the samples don’t have to be cooled. The experiments can therefore be conducted at room temperature, allowing the water network inside the proteins to be observed in a realistic, dynamic state.

A group of researchers headed by Müller-Werkmeister has already had some success with this method, studying an enzyme from a bacterium that occurs in contaminated

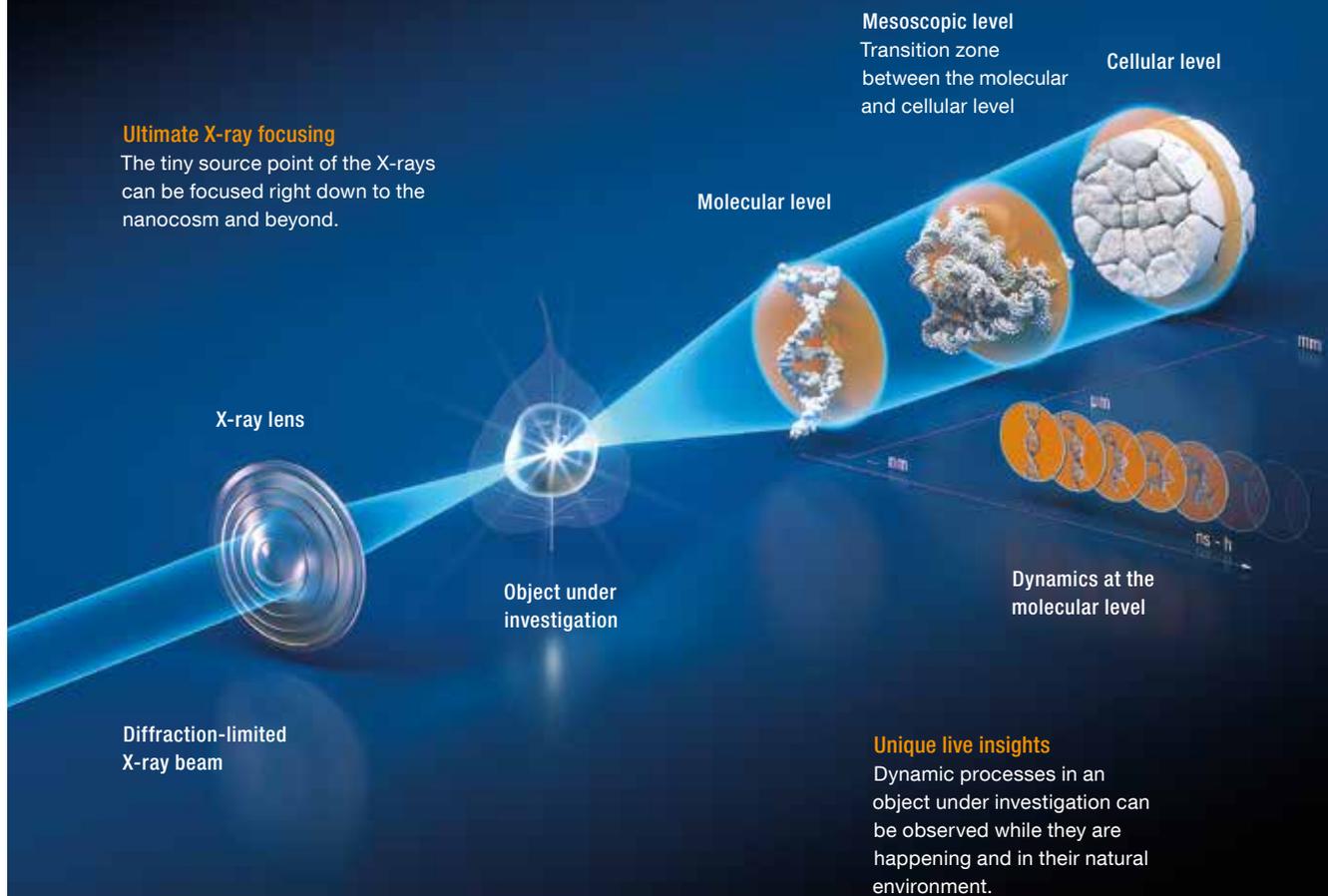
soil, for example. “We were surprised at the role that water played in this,” she says. The team was able to watch, in a kind of molecular film, how information was transferred between two subunits of the enzyme: not, as originally assumed, mechanically, like between intermeshing cogwheels, but along a “telephone line” consisting of four water molecules.

### Water in medicine

According to Müller-Werkmeister, “It may be a fundamental principle that certain protein reactions are regulated by such water networks. We want to investigate this further in the future, especially in the context of the new >>

**New dimension in imaging**

Real objects can be captured in sharp detail, on scales ranging from millimetres to nanometres.

**PETRA IV – the ultimate X-ray microscope**

The 3D X-ray microscope PETRA IV that is being planned at DESY will offer unique possibilities for deciphering the structure and dynamics of water in the requisite detail. This could lead to essential discoveries in the natural and life sciences, technology and healthcare.

In medical research, for example, PETRA IV will allow the individual movements of proteins measuring only a few nanometres across to be tracked live in living cells. The X-rays produced by PETRA IV can be dosed so precisely that biological samples do not suffer any radiation damage during the measurements. And the process of splitting water molecules to obtain hydrogen as an energy carrier can be observed on the nanoscale at PETRA IV in the immediate vicinity of catalyst particles used for that purpose. The insights can help to tailor catalysts optimised for splitting water.

At PETRA IV, water can be studied at unprecedented resolution in order to understand biological and chemical processes.

# “Watching water molecules as they dance”



The physicist Anders Nilsson is one of the best known water researchers in the world.

**Anders Nilsson:** To my mind, DESY is the ideal home for such a centre, because it offers extremely powerful X-ray sources, such as PETRA III and the European XFEL. And I believe that investigations using high-intensity X-ray pulses can reveal lots of new details about the nature of water. That infrastructure makes DESY an excellent site for a water centre.

**femto:** What kind of research would you personally like to do at the CMWS?

**Anders Nilsson:** Up until now, we have mainly been studying the static properties of water, taking still images, so to speak, and analysing them. But water is of course incredibly dynamic. Its molecules are constantly in motion, figuratively speaking they are performing a wild dance. Existing methods essentially allow us to observe how the water molecules behave before and after their dance. But if we want to really understand water, we need to find out what happens in between; we have to watch the molecules dance. The European XFEL and PETRA III will allow us to study these dynamics. And that's precisely the next step to a really fundamental understanding.

**A**nders Nilsson from the University of Stockholm is one of the world's most renowned water researchers. He proposed the idea of an interdisciplinary water centre in 2015, together with DESY Director Helmut Dosch. Nilsson gave the initial exchange of ideas a clearer shape by putting forward a two-page concept. He himself is hoping to explore the rapid inner dynamics of water at the new centre.

**femto:** What is the mission of the Centre for Molecular Water Science (CMWS)?

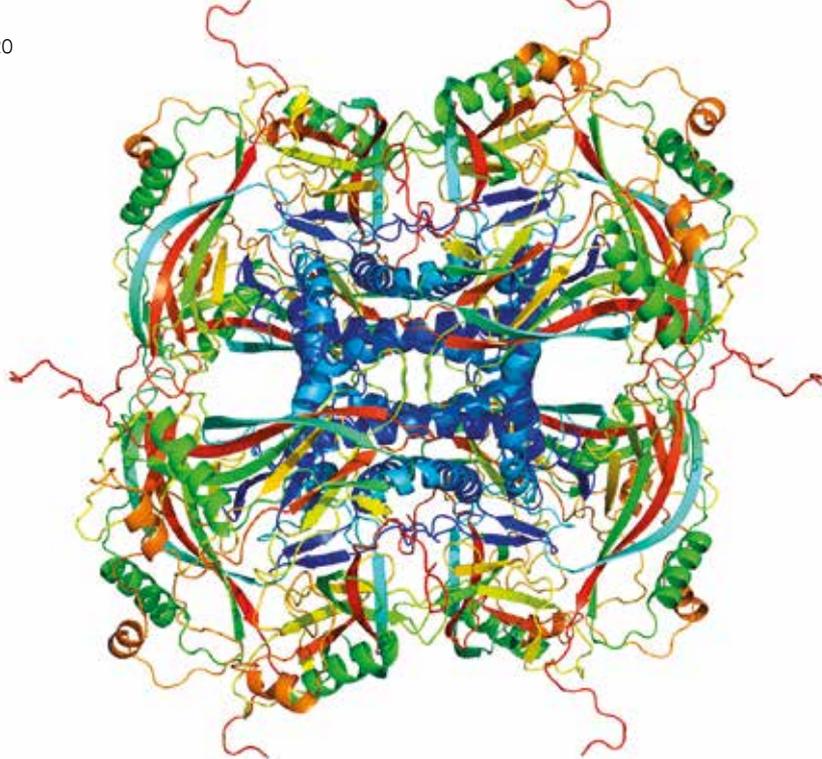
**Anders Nilsson:** Water is everywhere. It plays a role in a wide range of contexts – for life, for the environment, for the climate and for energy production. That's why I believe it's an excellent idea to study water from many different angles, at an interdisciplinary centre. So far, the amount of communication between the various research disciplines that are examining water has been very limited.

A joint water centre can overcome this and bring about a valuable transfer of knowledge. There is something of a vacuum in this respect in Europe. And the CMWS can fill that vacuum.

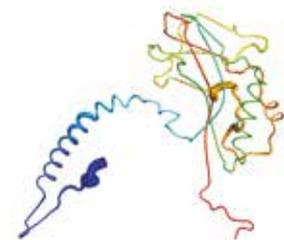
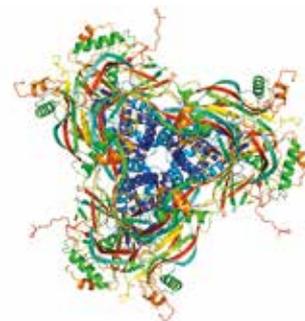
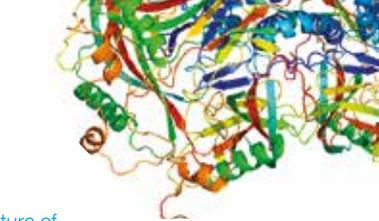
**femto:** What hopes do you have for this centre?

**Anders Nilsson:** Generally speaking, the aim is to develop a substantially deeper understanding of water. After all, water will be one of the key issues of the future. Take climate change, for example: This is going to have a very strong impact on water in terms of rising sea levels and changes in cloud cover, for example. The same is true of energy production: Up to now, oil has been considered the foundation of our society. In the future, water is likely to assume that role, in fuel cells or artificial photosynthesis, for example.

**femto:** The CMWS is to be set up at DESY. Is that a sensible idea?



The spatial structure of proteins can be deduced from the characteristic diffraction patterns they produce when exposed to X-rays.



*“Such fundamental knowledge is needed so that the pharmaceutical industry can make further progress in the future”*

Arwen Pearson, Universität Hamburg

water centre at DESY.” But there are other topics on the research agenda too: How does water affect the functionality of so-called unfolded proteins? These are abundant in all cells, and analysing them could reveal novel mechanisms for new drugs.

Water fulfils important functions for medicine outside the body too, for example as a solvent for new active pharmaceutical ingredients based on proteins or peptides. “These biomolecules are not very stable and become ineffective if they are not stored properly,” says Arwen Pearson, a biophysicist at Universität Hamburg. “This is particularly relevant in developing countries, where it can be difficult to keep medicines refrigerated at all times.”

The stability of a protein depends, among other things, on the solvent used. If there is not enough water, it can simply dry out. If there is only water present, the protein could unfold too much and become less stable as a result. “Adding small amounts of salts, for example, could prevent this,” explains Pearson. “So it’s very important to prepare the solvent appropriately.” Future experiments at the CMWS

will provide a crucial basic understanding of how biomolecules and water interact with each other. “Such fundamental knowledge is needed so that the pharmaceutical industry can make further progress in the future,” says Pearson.

The CMWS will also address a field of great topical interest: the role of water molecules in viral infections, such as those caused by the new coronavirus. The latter can only exist in water. When the virus dries out, it quickly perishes. Among other things, the new water centre will investigate how water molecules interact with the virus envelope and how water affects protein structures during the infection process. The work carried out at the new water centre could also assist the development of new active ingredients, so-called antivirals – for example by embedding these drugs in special water-based carriers. >>

The biophysicist Arwen Pearson from Universität Hamburg heads the Hamburg Advanced Research Centre for Bioorganic Chemistry (HARBOR).



Cosmic snowline: The temperature on the outskirts of the gas and dust disks orbiting young stars drops low enough for water ice to form. The radio telescope array ALMA has observed this snowline in the young star V883 Orionis (artist's impression).



### Water in space

Other water experts are looking much further afield – into space; because space exhibits an amazing chemical diversity. To date, special telescope techniques have identified more than 200 different types of molecules floating around in space – including some very complex ones, such as precursors of amino acids. The question is, how could these compounds have formed in the first place? This in itself is a mystery, because the prevailing temperature in many regions of space is extremely low and therefore not conducive to chemical reactions. On top of this, outer space is fairly empty. The virtually endless expanses between stars contain very few potential reactants. The probability of their meeting and undergoing a reaction is extremely low.

The answer to this riddle might have something to do with water. “Today, we believe that most of the reactions that occur in interstellar space take place on the surface

*“Today, we believe that most of the reactions that occur in interstellar space take place on the surface of ice particles”*

Melanie Schnell, DESY

of ice particles,” says Melanie Schnell, a leading scientist at DESY and also coordinator of the CMWS. The idea is that over time these molecules encounter roaming granules of ice and stick to them. Here, stimulated by ultraviolet radiation, for example, they can react with other molecules that have also been captured by the ice fragment. Eventually, the products formed in the reaction may then evaporate again. Some experts even speculate that some of the basic building blocks of life were created in this way.

“We are carrying out special experiments to find out how molecules can be created on such ice particles,” says Schnell. One of these experimental setups – a vacuum chamber operating at extremely low temperatures – simulates the prevailing conditions in space inside the laboratory. In this chamber, the scientists apply water to a substrate by vapour deposition to produce a thin layer of ice. A smidgeon of other molecules is also present, such as formaldehyde.

To trigger a chemical reaction, the team irradiates the formaldehyde-spiked ice surface with high-energy ultraviolet radiation. The resulting events can then be observed using infrared radiation, for example, or, as planned for the future, using microwaves. The spectral analysis of the radiation reveals which molecules have formed in the space simulator. “Among other things, we are looking to see whether any biologically relevant substances are produced,” says Melanie Schnell. “If we find any, this would be another important indication that ice in space does indeed act as a kind of interstellar catalyst.”

### Ortho-water and para-water

Another curious property that might be important for astrochemistry resides in the atomic nuclei of the water molecule, specifically in the two hydrogen nuclei. Like other atomic nuclei, these have a kind of intrinsic quantum mechanical angular momentum known as “spin”. Figuratively speaking, the nuclei align themselves like tiny spinning tops, pointing either up or down. The key point is that they interact differently with each other depending on the orientation of their nuclear spins. “This means that water can be in different quantum states in terms of these nuclear spins,” explains DESY physicist Jochen Küpper. “We call these ortho-water and para-water.”

Simply put, the two forms differ in terms of their internal energy content: Para-water has a quantum hint less energy than ortho-water and is therefore the ground state. As a result, if a glass of water, which at room temperature consists of three parts of ortho-water and one part of para-water, were cooled to well below minus 200 degrees Celsius, the para-form would steadily increase – nature always tends towards the lowest energy state. >>



femtopolis

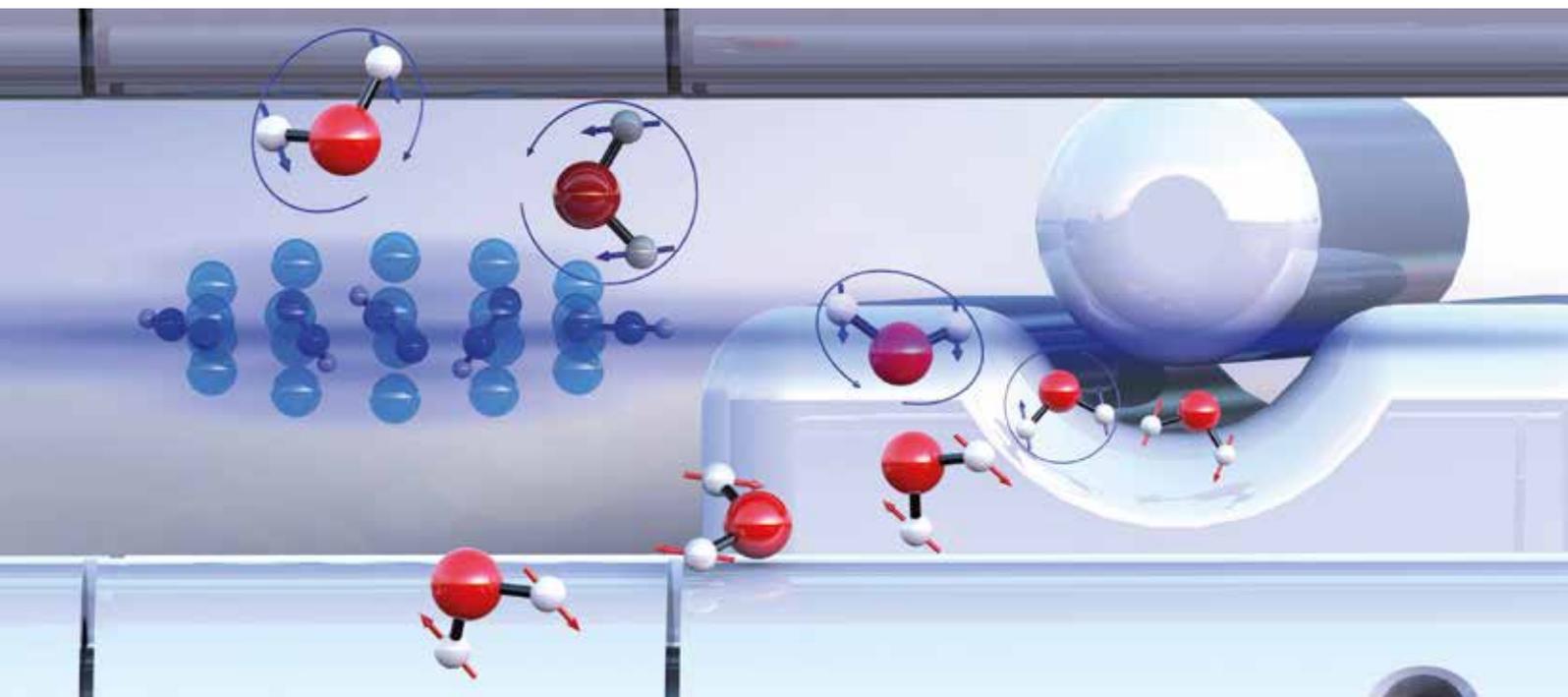
## Life without water?

Life is not possible without water. All life processes as we know them are based on the presence of water, the elixir of life. Although some life forms can survive extreme drought, they only come back to life when water is available again. And elsewhere in the universe? In their search for exotic alternative forms of life, astrobiologists have been examining Saturn’s moon Titan, for example. Titan has a dense atmosphere, consisting mainly of nitrogen, and a liquid cycle that includes clouds, rain, evaporation and lakes on its surface. However, the stuff that flows around on Saturn’s moon is not water but liquid gas, more specifically liquid methane and ethane. In principle, this could assume the biological functions of water, and similar conditions are also conceivable on other celestial bodies.

However, at average temperatures of minus 180 degrees Celsius, the type of biological cells that we know on Earth would not stand a chance on Titan. In particular, lipid membranes, the protective sheaths that hold together living cells on Earth and prevent their contents from simply leaking out into the surrounding water and drifting away, cannot form. Astrobiologists have come up with an alternative, though, the so-called azotosome, a cell membrane based on nitrogen compounds. The azotosome works like terrestrial lipid membranes and could be composed of the compound acrylonitrile in particular. In 2017, just two years after the idea of the azotosome was first proposed, researchers actually discovered acrylonitrile on Titan using the ALMA radio telescope array in the Chilean Andes. However, so far there are no signs of exotic unicellular organisms on the icy moon.

In fact, biological cells might have a hard time on Titan despite the azotosome. Theoretical considerations suggest that while this alternative cell membrane would be stable under the conditions found on Titan, it would not be able to form in the first place, at least not by itself: In the absence of any external influences, acrylonitrile simply freezes to become ice. However, this does not necessarily spell the end for hypothetical aliens on Titan. Scientists suspect that at the low temperatures found on Saturn’s moon, cells might actually be more like solids rather than a loose collection of organelles suspended in a liquid. Such cells would depend on small molecules such as acetylene diffusing into them from the surrounding liquid hydrocarbon soup – so a cell membrane might even get in the way.

Either way, the idea is certainly inspiring and could lead to new models and perhaps even to the discovery of extraterrestrial life forms that manage entirely without water and have found fascinating ways of using other molecules in their life processes.



Ortho-water and para-water molecules with different spins (blue and red arrows, respectively) react at different rates with other substances, such as diazenylium ions (centre left).



Jochen Küpper is the head of the Controlled Molecule Imaging group at the Center for Free-Electron Laser Science (CFEL) at DESY.

The question is: To what extent do these two varieties differ in their behaviour towards other substances? To answer this, Küpper and his team first had to overcome a difficult hurdle – they had to separate the ortho-water and para-water. “To do this, we produce a jet made up of individual water molecules,” Küpper explains. “We send them through a special electric field that deflects the molecules upwards.” The trick is that the ortho-water and para-water molecules are deflected by different amounts and thereby separated from each other. “We split the molecular beam into several distinct beams, just like a prism splits sunlight into all the colours of the rainbow,” says Küpper. “This is why we call our device an electric prism.”

The researchers then directed the ortho-water and para-water molecules into electrical traps, where a reactant was waiting for them:  $N_2H^+$ , a nitrogen compound. On coming in contact with the water, the ion transferred a hydrogen nucleus to the water molecule. The products of the reaction were molecular nitrogen and the “acid molecule”  $H_3O^+$ . As a result, “We found that para-water reacts 25 percent faster than ortho-water,” explains Jochen Küpper. “This means that para-water and ortho-water are actually two different molecules, which came as quite a surprise to chemists.”

The result is relevant for astrochemistry. Individual water molecules are constantly evaporating from the tiny ice crystals that are found in space. The suspicion is that the molecules that have evaporated gradually

heat up over time – with the exception of the spins of their hydrogen nuclei, which retain their original ice temperature for a very long time. “This would explain why we always find more para-water than expected in space at higher temperatures,” says Küpper. “And this then sometimes reacts more quickly with other molecules than ortho-water.” That could have implications for the models proposed by astrochemistry, for example.

*“This means that para-water and ortho-water are actually two different molecules, which came as quite a surprise to chemists”*

Jochen Küpper, DESY

### Water in energy production

Water is likely to play a central role in the energy supply of the future, especially as a starting material for producing green hydrogen. To achieve this, water molecules must be split using energy from renewable sources. Nowadays, this is mainly done by electrolysis in several stages. First, wind turbines or solar cells generate climate-neutral electricity, which is then fed into a system that electrically separates the water into its components. >>

# “We are overwhelmed by the Europe-wide interest”

The time is ripe for a water centre, says DESY Director Helmut Dosch

**femto:** DESY is planning to set up a centre that will focus on research into water. What are your motives?

**Helmut Dosch:** Water is essential for life on Earth. It plays a vital role in the environment, in biology and medicine. But it is also crucial for technology: Many catalytic processes take place in an aqueous environment, and every year corrosion causes a tremendous amount of damage. So we would do well to understand water in as much detail as possible. To do so, we need to study its behaviour at the molecular level. Only then can we get to the bottom of its distinctive characteristics, such as the anomaly of its having its greatest density at four degrees Celsius. At DESY, we operate the research tools that are necessary for such investigations: ultra-modern X-ray sources that can be used to capture the extremely fast movements of water molecules as snapshots, for example. That’s why we’re addressing the topic now.

**femto:** How did the idea arise in the first place?

**Helmut Dosch:** At DESY, we have experts who have been working on the subject for quite some time. But others have also been involved from the very beginning, most notably the physicist Anders Nilsson from Stockholm. Then we sent up a trial balloon: We wrote to all kinds of people in Europe and invited them to attend a brainstorming workshop in

Helmut Dosch has been the chairman of DESY’s Board of Directors since 2009.



Hamburg, to see how great the interest was among scientists. The response was tremendous, we were overwhelmed. In the meantime, the project has developed to become an impressive European initiative. To date, more than 40 institutions have declared a desire to become involved in the Centre for Molecular Water Science (CMWS), also financially. So it seems that the time is ripe for a water centre.

**femto:** How relevant is the CMWS for the economy and for society?

**Helmut Dosch:** It is mainly a matter of fundamental research and finding answers to fundamental questions. But if we find these answers, they could be important for many practical applications. Think of corrosion control or catalytic reactions in aqueous environments, for example. Getting to grips with those would have huge economic benefits. Environmental

aspects are important too, for example with regard to drinking water. Specific molecular filters are needed to remove residues of drugs and hormones from water. Another important aspect that has recently gained enormously in importance is a detailed molecular understanding of viral and bacterial processes in aqueous environments – this affects human beings as well as the environment. The CMWS could lay important foundations for all of this.

**femto:** What is the next step for the water centre?

**Helmut Dosch:** We have issued a policy paper that describes exactly how we intend to advance molecular water research, and this has generated enormous interest at the national and international level. The first pilot projects have already begun. We are extremely optimistic that the centre will be set up in the near future.



Simone Techert is a leading scientist at DESY.

*“We are working with the research department of a large automotive company, among others, to try and develop practical implementations”*

Simone Techert, DESY

However, a single-step procedure – known as photocatalytic water splitting – is likely to be much more effective: In this process,  $H_2O$  is split directly by light, without any detours.

For this to work, a molecular assistant is needed: a catalyst that substantially speeds up the dissociation of the water molecule and thus makes the reaction possible in the first place. “So-called perovskites seem to be suitable for the task, for example,” says DESY scientist Simone Techert. “This is a class of materials that could also be of interest for future solar cells.” However, a number of aspects still needs to be studied before the technology can be applied. What composition of materials is best suited for splitting water, especially if water comes into direct contact with the catalyst? How can these materials be produced in a cost-effective and environmentally friendly way, preferably as an aqueous solution? How well will they keep? And can they be recycled easily?

To find answers, Techert’s team is planning to conduct a number of experiments, including at the European XFEL. There, the experts want to direct laser pulses at crystals of catalysts wetted with water so as to trigger water splitting. They

will then use ultrahigh-power X-ray pulses to analyse in detail what happens when the water molecules are split and how this process can be optimised. “This is not just about fundamental research,” Simone Techert points out. “We are working with the research department of a large automotive company, among others, to try and develop practical implementations at some time in the future.”

### Water as climate regulator

Another area in which water is of prominent importance is the climate. The oceans, for example, are active players when it comes to our climate. They store large amounts of heat and  $CO_2$ . The Earth’s atmosphere also contains a lot of water: up to four percent, depending on the latitude and on weather conditions. Clouds – huge conglomerations of water droplets and tiny ice crystals – are particularly relevant to the climate. However, the precise extent of their influence on global warming is one of the biggest uncertainties in current climate models. Will clouds further fuel climate change as temperatures rise? Or could they mitigate the effect and thus defuse things a little?

To answer these questions, experts are painstakingly analysing the way in which clouds are formed. “Tiny particles are suspended in the air, the smallest just a few nanometres, the largest up to 100 micrometres across,” explains Nønne Prisle, an atmospheric scientist at the University of Oulu in Finland. “Water vapour can condense on these airborne particles to form droplets.” These particles are essential in order for clouds to form. If the air were surgically clean, the atmosphere would have to be far more humid in order for cumulus and cirrus clouds to form.

Some 200 scientists from 40 countries came to DESY for the “Water Week” to discuss the interdisciplinary CMWS and move it forward.





Preparing to investigate the details of cloud formation using X-rays

“As soon as a water droplet condenses on a particle, it can dissolve certain components of that particle, such as soap-like organic molecules,” Prisle explains. “So the droplet does not consist of pure water, but is actually a highly complex solution.” The key point is that the dissolved molecules can drastically alter the way the droplet behaves. They throng to its surface, alter the surface tension and thereby stabilise the droplet, thus ultimately increasing cloud formation.

*“Up until now, I have often felt somewhat isolated, like some kind of water nerd. The CMWS would be full of like-minded people, and I would find that very inspiring.”*

Nønne Prisle, University of Oulu

To study these processes in more detail, Prisle’s team uses the ultrahigh-intensity X-ray pulses produced by particle accelerators such as PETRA III. The scientists fire a supersonic jet of water enriched with organic molecules into a vacuum chamber. When an X-ray pulse collides with this solution, it can strip away electrons, which are then captured by a detector. Analysing the measured data reveals the arrangement of the molecules on the surface of the water. “If you keep increasing the concentration of organic molecules in the water, the surface of

the water will eventually become saturated,” explains Prisle. “You simply cannot fit in any more molecules.

But what effect do these phenomena have on cloud formation and thus on the climate? Nønne Prisle estimated this some time ago by means of a computer simulation. “The change in the surface tension should increase cloud formation and thus have the effect of cooling the atmosphere,” she says. “This effect could be substantial.” If the experts are right, this could have unpleasant consequences in the future: Some of the airborne particles that serve as condensation nuclei for clouds are man-made and are introduced into the atmosphere by traffic and industrial emissions. In principle, it is important to reduce this air pollution because it costs thousands of lives every year. But while cleaner air would be good for people’s health, it would reduce cloud formation and thus the cooling effect this produces – global warming would be accelerated.

However, such forecasts are still subject to various uncertainties. In order to make them more precise, Prisle’s group is now planning new, more sophisticated experiments. She is working on a sample system that produces a steady stream of tiny droplets instead of a fine jet of water, which can then be examined using X-rays. Nønne Prisle would love to conduct such experiments in the context of the planned water centre. “This is a fantastic initiative,” she says.

“Up until now, I have often felt somewhat isolated, like some kind of water nerd. The CMWS, on the other hand, would be full of like-minded people, and I would find that very inspiring.”



Nønne Prisle is an atmospheric scientist at the University of Oulu in Finland.

# The ultrafast birth of free radicals

X-ray flashes provide unrivalled insight into the first rapid chemical reaction during the radiolysis of water

Using extremely short X-ray flashes, an international team of researchers has for the first time ever observed details of the ultrafast chemical reaction leading to the formation of aggressive radicals when water is irradiated. The study provides unprecedented insights into the fastest chemical reaction in this process, which can lead to radiation damage in the body, but is also very important in other fields such as materials science.

The researchers investigated the radiolysis of water, as scientists call the splitting of a chemical compound – in this case water – by radiation. “Our body consists essentially of water,” explains DESY scientist Robin Santra, one of the leaders of the study. “We are all exposed to ionising radiation in everyday life – whether through X-rays, natural radioactivity or, for example, cosmic radiation on air travel. Therefore, what happens here is of fundamental importance.”

In the radiolysis of water, high-energy radiation first knocks an electron out of a water molecule ( $\text{H}_2\text{O}$ ), thereby ionising it to  $\text{H}_2\text{O}^+$ . This is followed by a so-called proton transfer, in which the ionised water molecule releases a hydrogen nucleus (proton) to an adjacent molecule. This produces an extremely reactive hydroxyl radical (OH), which can cause damage in the organism, and a hydronium ion ( $\text{H}_3\text{O}^+$ ). The process itself has been known for a long time, but how it takes place had not been observed in detail – partly because it is extremely fast.

“The truly exciting thing is that we’ve witnessed the very fastest chemical reaction in ionised water, which leads to the birth of the hydroxyl radical,” says Linda Young from the Argonne National Laboratory in the USA, who led the research together with Santra and Zhi-Heng Loh from Nanyang University of Technology in Singapore. “The hydroxyl radical is itself of considerable importance, as it can diffuse through an organism, including our bodies, and damage virtually any macromolecule including DNA, RNA and proteins.” A deeper understanding of radiolysis could possibly help to develop strategies to suppress the formation of the hydroxyl radical.

*“We could show that the X-ray data actually contain information on the dynamics of the water molecules that enable the proton transfer”*

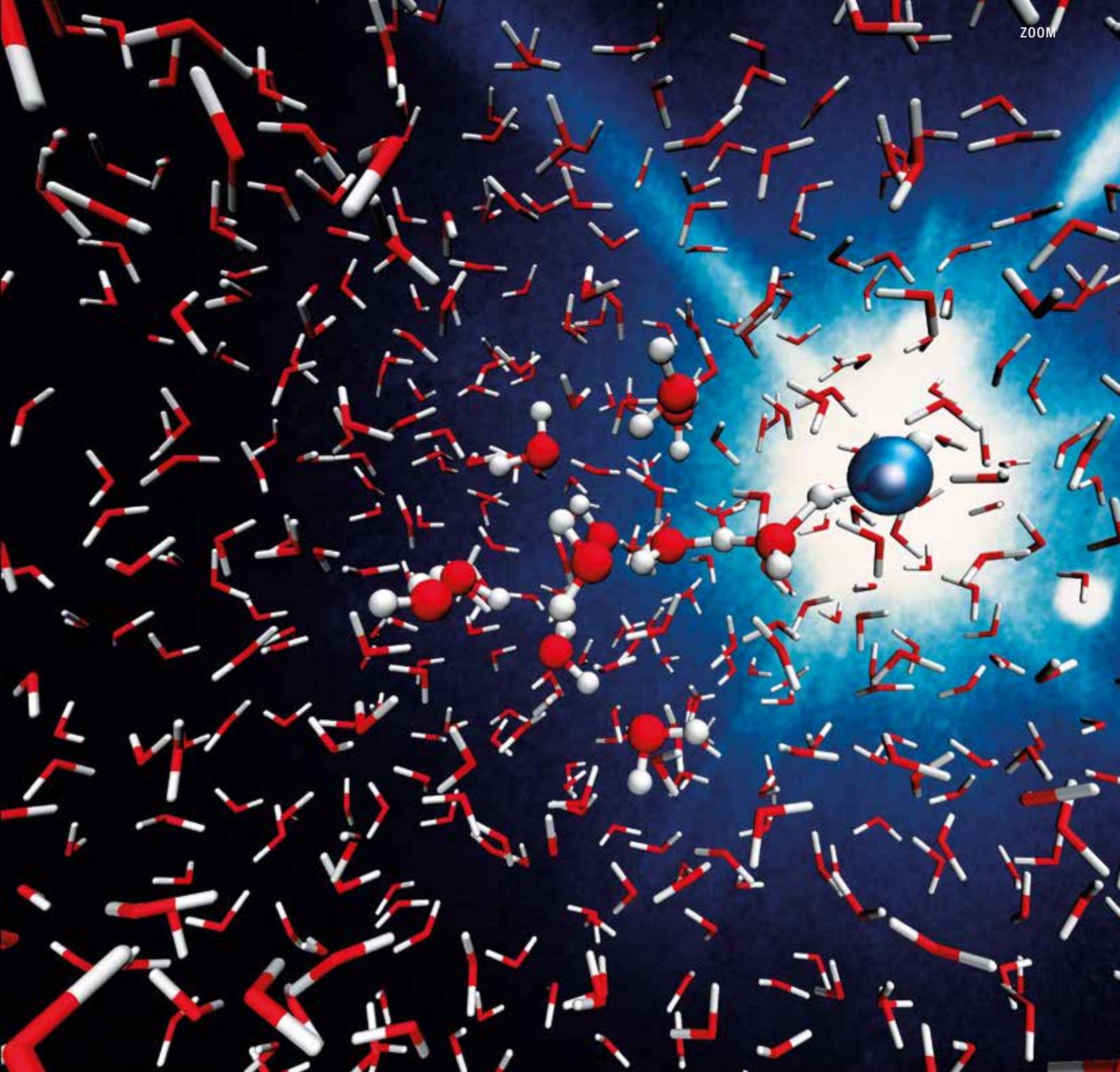
Robin Santra, DESY

For the investigation, the scientists ionised water by laser and then took extremely short snapshots of the processes triggered by the ionisation, using the LCLS X-ray laser at the SLAC National Accelerator Laboratory in California. The X-ray laser allows for ultrashort exposure times of only about 30 femtoseconds (quadrillionths of a second).

The detailed analysis of the measurement data confirms the theoretical modelling of the proton transfer done by Santra’s team at the Center for Free-Electron Laser Science (CFEL) at DESY. “We could show that the X-ray data actually contain information on the dynamics of the water molecules that enable the proton transfer,” says the DESY theorist. “In just 50 quadrillionths of a second, the surrounding water molecules literally move in on the ionised  $\text{H}_2\text{O}^+$  molecule until one of them comes close



Robin Santra heads the theory group at the Center for Free-Electron Laser Science (CFEL) at DESY.



enough to grab one of its protons in a sort of handshake, turning into hydronium  $\text{H}_3\text{O}^+$  and leaving behind the hydroxyl radical  $\text{OH}\cdot$ ." According to the observations, this proton transfer typically takes place in only 46 quadrillionths of a second.

The researchers have thus succeeded in taking a first decisive step towards clarifying the extremely fast dynamics of the radiolysis of water. "Our recent work shows that the fastest chemical reaction in ionised water occurs on the 50 femtoseconds time scale," summarises Loh. "While 50 femtoseconds might already

seem short by most standards, there are still many physical processes within these 50 femtoseconds that remain unobserved. The ultimate goal is to uncover the intricate network of physico-chemical processes that occur in ionised liquid water, starting from the time that ionising radiation impinges upon water to the birth of the highly reactive  $\text{OH}\cdot$  radical."

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*Science, 2020; DOI: 10.1126/science.aaz4740*

The illustration shows the moment of proton transfer from an ionised to a neutral water molecule, resulting in the formation of a hydroxyl radical and a hydronium ion. The blue cloud shows the orbital from which the electron was knocked out by irradiation.

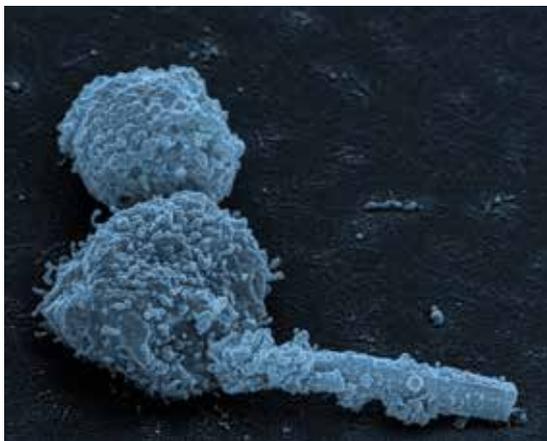
# Science in brief

## New approach for sleeping sickness drugs

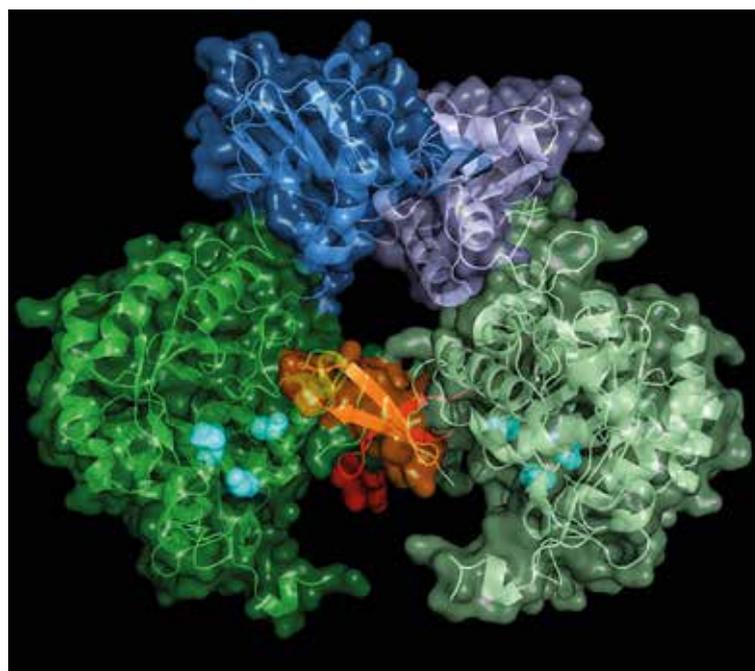
**S**leeping sickness is caused by the parasite *Trypanosoma brucei*, which is transmitted by the bite of the tsetse fly, endemic in southern Africa. The infection is considered one of the most significant tropical diseases.

In the search for a possible starting point for drugs against the pathogen, a team led by Christian Betzel from Universität Hamburg, Lars Redecke from the University of Lübeck and DESY and Henry Chapman from DESY decoded the detailed spatial structure of a vital enzyme of the pathogen. The result provides a possible blueprint for an active substance that specifically blocks this enzyme and thus kills the pathogen.

In order to analyse the enzyme, known as inosine-5'-monophosphate (IMP) dehydrogenase, the researchers induced certain insect cells to crystallise the enzyme inside them. The tiny, needle-shaped crystals were analysed with the LCLS X-ray laser at the US research centre SLAC in California. The team recorded the diffraction patterns of more than 22 000 microcrystals and was able to calculate the



The microcrystals grow in needle-shaped rods protruding from the insect cells that produce them.



Structure of the parasite's IMP dehydrogenase: The active enzyme forms pairs (dimers). The "switch" region (Bateman region) is shown in shades of blue.

spatial structure of the enzyme with an accuracy of 0.28 millionths of a millimetre (nanometres), which corresponds roughly to the diameter of an aluminium atom. "The result does not only show the exact structure of the enzyme switch, the Bateman region, but also which molecules of the cell activate the switch and how these so-called co-factors bind to the enzyme switch," reports Karol Nass from DESY. The data might provide an approach for inhibiting the parasite's IMP dehydrogenase.

*Nature Communications*, 2020;

DOI: 10.1038/s41467-020-14484-w

# Novel material with high-tech prospects

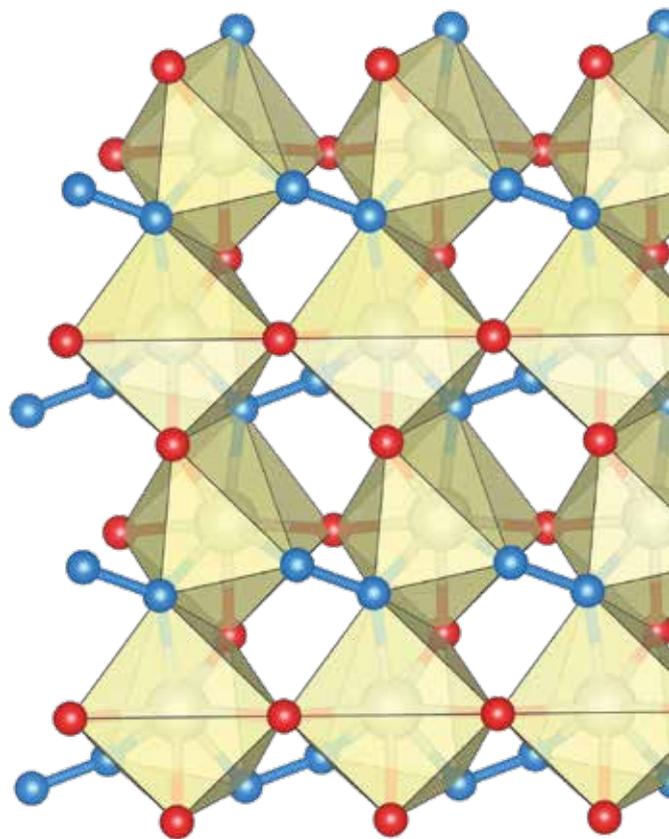
**A**n international research group led by scientists from the University of Bayreuth has identified a previously unknown material at DESY: rhenium nitride pernitride. Thanks to a combination of properties that were previously considered incompatible, it looks set to become highly attractive for technological applications. The new material is a superhard metallic conductor, which can withstand extremely high pressures like a diamond. The manufacturing process developed in Bayreuth can also be applied to other technologically interesting materials.

The possibility of finding a compound that was metallically conductive, superhard and ultra-incompressible was long considered

unlikely. Scientists believed that these properties could not occur simultaneously in the same material and were therefore incompatible. This assumption has been refuted by the research work now published, which was carried out at DESY's X-ray source PETRA III, among others.

At present, the exact scope of application for the new material is still difficult to define, but its exceptional combination of attractive physical properties makes rhenium nitride pernitride a material that can help meet the technological challenges of the future.

*Nature Communications*, 2019;  
DOI: 10.1038/s41467-019-10995-3

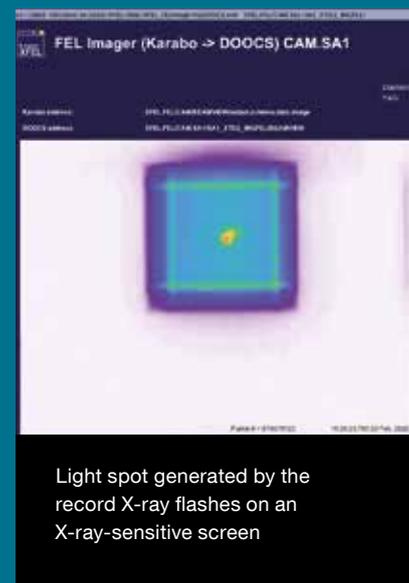


The structure of rhenium nitride pernitride, containing single nitrogen atoms (red) and nitrogen dumbbells N-N (blue). Larger spheres show rhenium atoms.

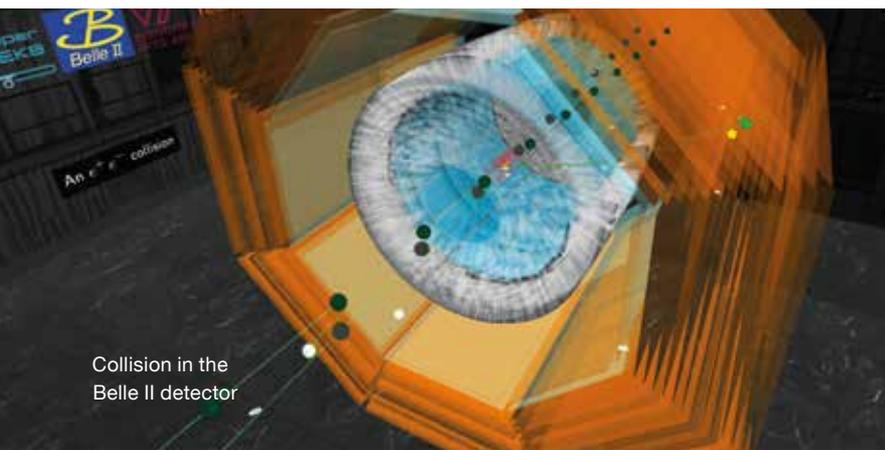
## European XFEL generates laser light with record energy

**T**he European XFEL X-ray laser has set a new energy record for the generated X-ray radiation: As the only X-ray free-electron laser worldwide, it is now able to produce intense X-ray flashes with an energy of 25 kiloelectronvolts per light particle (photon), enabling scientists to venture into uncharted worlds and investigate complex phenomena like never before.

Hard, short-wavelength X-ray radiation in ultrashort pulses of less than 100 quadrillionths of a second (femtoseconds) duration, such as those generated by the European XFEL, open up unprecedented scientific opportunities to probe matter and materials at the atomic level on ultrashort time scales. With a photon energy of 25 kiloelectronvolts (keV), corresponding to a laser wavelength of 0.5 angstroms (0.05 nanometres), the DESY team operating the European XFEL accelerator set a new wavelength record for laser light. In addition, by changing the setting of the SASE1 undulator, one of the light generation devices of the European XFEL, the accelerator team was able to push the limit even further to 30 keV, observing clear indications of free-electron laser radiation on a scintillating screen.



Light spot generated by the record X-ray flashes on an X-ray-sensitive screen



Collision in the Belle II detector

## In search of the Z' boson

About one year ago, the Belle II detector went into operation at the Japanese research centre KEK. Now, the international Belle II collaboration of scientists published the first results obtained with the help of the detector. The publication sets some limits to the properties of a new particle related to dark matter. According to current

knowledge, dark matter is more than five times more common in the universe than the matter we are familiar with.

Scientists at 12 institutes in Germany are involved in the construction and operation of the Belle II detector. DESY plays a leading role, especially in the integration and commissioning of the highly sensitive innermost detector, the pixel vertex detector. In addition, the German groups are involved in the development of evaluation algorithms and in the data analysis.

With Belle II, researchers are looking for hints of new physics that can be used, for example, to explain the unequal relationship between matter and antimatter, or the mysterious dark matter. One of the so far undiscovered particles that the scientists are searching for with the Belle II detector is the Z' boson – a variant of the photon (particle of light), which, unlike the photon, has mass. It could play an interesting role in the interaction between dark and normal, visible matter, i.e. it could act like a kind of mediator between the two forms of matter.

*Physical Review Letters, 2020;*  
DOI: 10.1103/PhysRevLett.124.141801

Picture: KEK, Belle II, Zachary Duer, Tanner Uptegrove, Leo Pillonen, George Glasson, W. Jesse Barber, Samantha Spytek, Christopher Dobson (Virginia Tech Institute for Creativity, Arts and Technology, Virginia Tech Department of Physics, Virginia Tech School of Education)

## How molecular footballs burst in an X-ray laser

An international research team has observed in real time how football molecules made of carbon atoms burst in the beam of an X-ray laser. The study shows the temporal course of the bursting process, which takes less than a trillionth of a second, and is important for the analysis of sensitive proteins and other biomolecules, which are also frequently studied using bright X-ray laser flashes. The football molecules disintegrate more

slowly and differently than expected, as the team around Nora Berrah from the University of Connecticut (USA) and Robin Santra from DESY discovered.

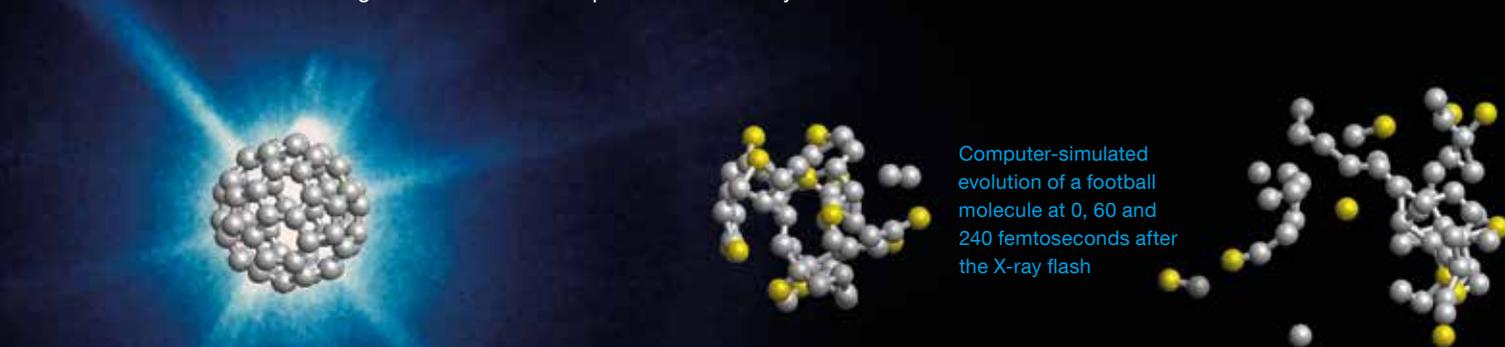
The researchers had experimented with buckminsterfullerenes, or buckyballs for short. These are well suited as a simple model system for biomolecules. Since they consist of only one type of atom and have a symmetrical structure, they can be well represented in theory and

experiment. This is a first step before the investigation of more complex molecules made up from different types of atoms.

The results obtained lay the foundation for a deeper understanding and a quantitative modelling of the radiation damage in biomolecules induced by X-ray laser flashes, the scientists write.

*Nature Physics, 2019;*  
DOI: 10.1038/s41567-019-0665-7

Picture: DESY, Zoltan Jurek



Computer-simulated evolution of a football molecule at 0, 60 and 240 femtoseconds after the X-ray flash

# Milestone for miniature accelerator

Scientists at DESY have achieved a new world record for a miniature particle accelerator: For the first time, an accelerator powered by terahertz radiation more than doubled the energy of the injected electrons. At the same time, the setup made up of two coupled terahertz manipulators significantly improved the quality of

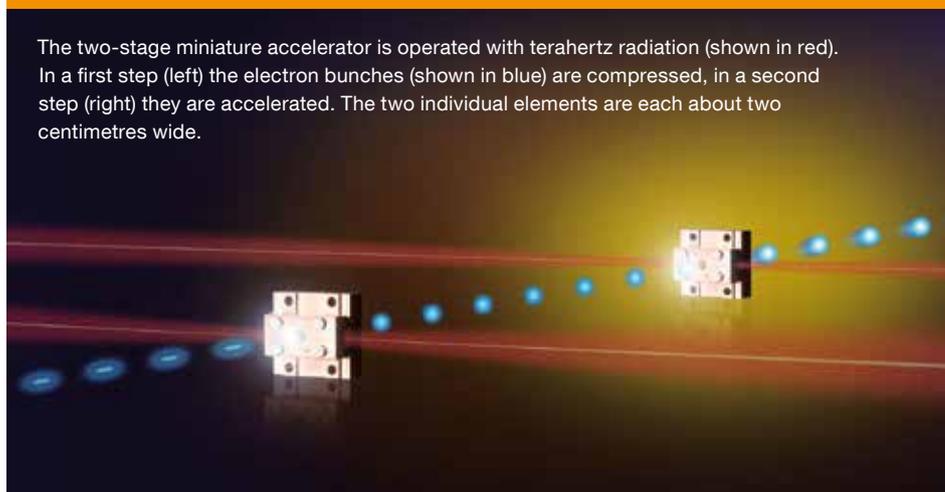
the accelerated electron beam compared to earlier experiments with the technique.

Terahertz radiation lies between infrared and microwave frequencies in the electromagnetic spectrum and promises a new generation of compact particle accelerators that open up new applications. The technology is

currently under development. The team around DESY researcher Dongfang Zhang has now built a two-stage accelerator. The first stage compresses the incoming electron bunches from about 0.3 to 0.1 millimetres in length, while the second accelerates the compressed bunches from 55 to 125 kiloelectronvolts.

“This is the first energy boost greater than 100 percent in a terahertz-powered accelerator,” emphasises Zhang. The coupled device produces an accelerating field (gradient) with a peak strength of 200 million volts per metre (MV/m) – close to that produced by the strongest state-of-the-art conventional accelerators.

*Optica*, 2019;  
DOI: 10.1364/OPTICA.6.000872



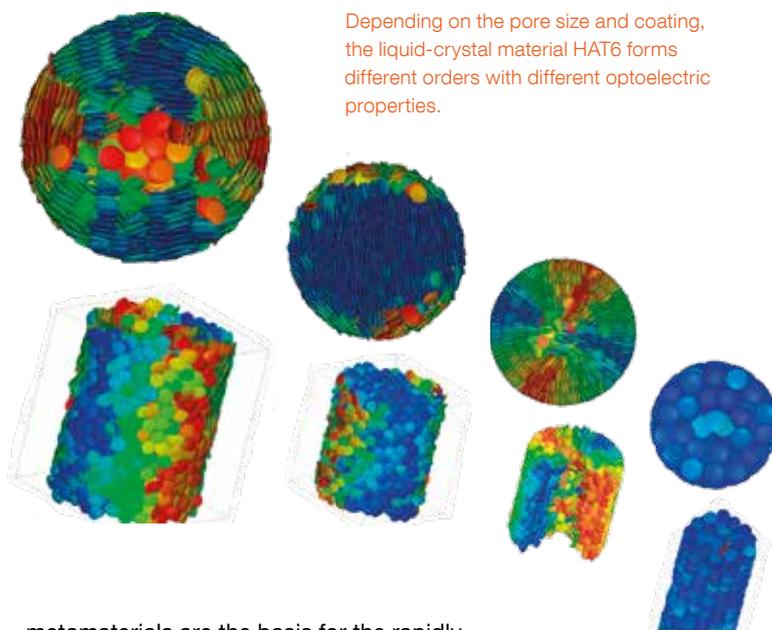
The two-stage miniature accelerator is operated with terahertz radiation (shown in red). In a first step (left) the electron bunches (shown in blue) are compressed, in a second step (right) they are accelerated. The two individual elements are each about two centimetres wide.

## Self-organisation of liquid crystals

Liquid crystals can arrange themselves in nanometre-sized pores in an amazing variety of ways. This self-organisation makes entirely new materials possible, as a team led by Patrick Huber from the Hamburg University of Technology reports. Using DESY’s X-ray light source PETRA III, among others, the researchers investigated how pore and material properties influence the order that the liquid crystals form.

The team used a liquid-crystal material consisting of disc-shaped molecules. By varying the size of the pores and using a hydrophilic or hydrophobic (water-attracting or water-repellent) coating of the pore wall, the researchers were able to control whether the disc-shaped molecules attached themselves to the pore wall with their flat side or their edges and which order they formed.

“The different collective orders of the liquid crystals have different electrical and optical properties,” explains Huber. “Such tailor-made and adaptive



Depending on the pore size and coating, the liquid-crystal material HAT6 forms different orders with different optoelectric properties.

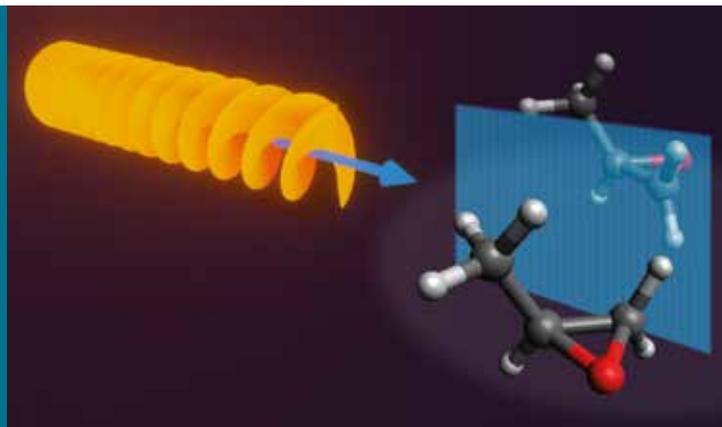
metamaterials are the basis for the rapidly developing transformative optics. Here, light paths can be realised in materials that are not possible with classical materials. Examples are extremely thin optical lenses with high refractive power, which could perhaps please any spectacle wearer in the future, or coatings that make objects invisible.”

*Nanoscale*, 2019; DOI: 10.1039/C9NR07143A

# Corkscrew laser separates mirror molecules

**A**n innovative approach can be used to separate the often occurring mirror-image versions of molecules. Many of the molecular building blocks of life exist in two versions that are mirror images of one another, which can exhibit completely different chemical behaviour. For example, one version of the organic compound carvone tastes like mint, but its mirror form tastes like caraway seed. In medicine, being able to distinguish between the two versions and to separate them can be vital.

Up to now, methods to separate mirror variants of molecules have mostly been designed for liquids. The approach developed by the group around DESY researcher Jochen Küpper is intended for gases. It is based on a special laser setup known as an optical centrifuge – a corkscrew-shaped laser pulse that excites molecules to ultrafast rotations. In addition, the laser is combined with an electric field.

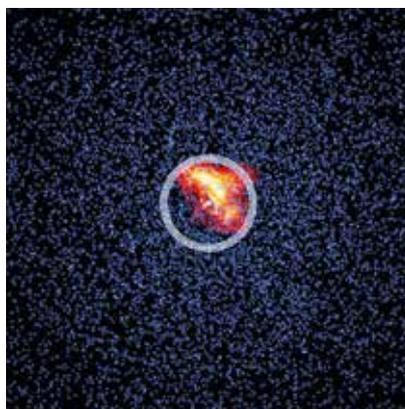


In this setup, mirror versions of molecules behave differently, enabling them to be spatially separated.

The researchers report that the enrichment in the respective variant can be controlled by simply changing the length of time during which the molecules interact with the laser field. The new method also creates a new theoretical framework for understanding the phenomenon of mirror-image molecules in nature.

The new approach proposes to combine a corkscrew-like laser pulse with an electric field to spatially separate mirror-image versions of chemical compounds.

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*Physical Review Letters*, 2019;  
 DOI: 10.1103/PhysRevLett.123.243202



The X-ray emission from the Crab Nebula as imaged with the Chandra telescope is shown in the centre in yellow/orange (image courtesy of M. C. Weisskopf and J. J. Kołodziejczak). The blue points denote the reconstructed directions of gamma-ray events as measured with the H.E.S.S. telescopes. The white circle shows the corresponding extension of the Crab Nebula as derived by the H.E.S.S. scientists.

# Supernova in gamma light

**T**he Crab Nebula is the remnant of a supernova in our galaxy that was observed almost 1000 years ago. Although it is one of the best-studied celestial objects, its extension in very-high-energy gamma rays remained unknown. Using the H.E.S.S. telescopes in Namibia, an international team of scientists has now succeeded in measuring the extension of the Crab Nebula in the very-high-energy gamma-ray range.

Gamma radiation from the Crab Nebula was first measured with ground-based telescopes in 1989. Until today, however, in gamma light, the supernova remnant could not be distinguished from a point source. The reason was the comparably poor angular resolution of the telescopes: They do not measure the gamma rays directly, but instead record particle

showers triggered when cosmic gamma quanta enter the Earth's atmosphere. From this measurement, it is possible to reconstruct the direction of origin of the original cosmic gamma quantum.

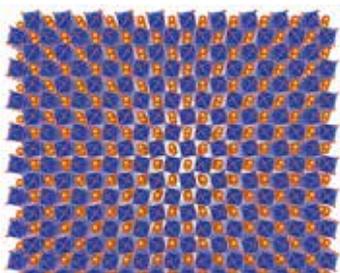
"For the first time, a novel simulation environment was used for this measurement, which takes into account the conditions when observing the Crab Nebula at an unprecedented level of detail," reports Stefan Ohm, head of the H.E.S.S. group at DESY. This has drastically increased the accuracy. The determined extension in gamma light agrees well with that measured in other wavelength ranges.

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*Nature Astronomy* 2019;  
 DOI: 10.1038/s41550-019-0910-0

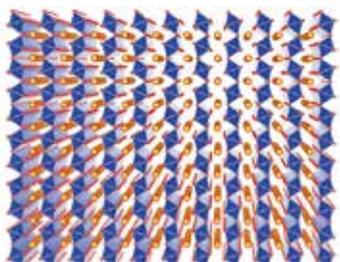
# View into Earth's deep mantle

**S**imulating the pressure conditions 2700 kilometres deep underground, an international research team has gained new insights into the properties of the most abundant mineral on Earth, bridgmanite. The measurements reveal how bridgmanite turns into a structure known as post-perovskite at the boundary to the Earth's core. Both forms have the same chemical composition, but a different internal structure. Since bridgmanite is the main component of the Earth's mantle, this structural transformation has significant effects on the dynamics in the lower mantle, including the propagation of seismic waves.

"We have known for 15 years that bridgmanite transforms into a different crystal structure called post-perovskite under these conditions," explains research leader Sébastien Merkel from the University of Lille in France. "What we didn't know was how fast it does that." At the Extreme Conditions Beamline at DESY's X-ray source PETRA III, the scientists were now able to investigate the dynamics of the transformation.



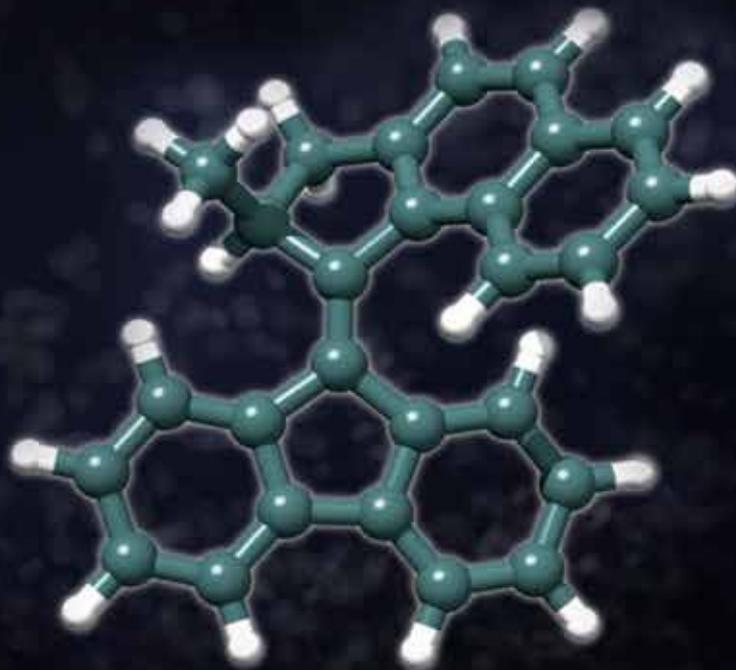
The crystal structures of bridgmanite (top) and post-perovskite (bottom)



It turned out that the conversion happens in about 10 to 10 000 seconds, depending on the pressure and temperature. "This means that seismic waves can trigger the transformation – and thus amplify the seismic signal," emphasises Merkel. "This observation explains why you sometimes see strong reflections and sometimes you don't. And it might also explain other anomalies."

*Nature Communications*, 2019; DOI: 10.1038/s41467-019-13482-x

femtomenal



# 47

**ATOMS** form the smallest machine that has

ever been operated at DESY: It consists of just one single molecule with 27 carbon atoms and 20 hydrogen atoms. Using microwaves, a team led by DESY researcher Melanie Schnell deciphered the exact structure of the artificial molecular motor, which had been synthesised by a team around Dutch Nobel laureate in chemistry Ben Feringa. Just like a large motor, the molecule has a rotor and a stator. The investigation revealed the arrangement of the individual parts of the mini-motor, which has a diameter of only 1.2 nanometres (millionths of a millimetre). Assuming for the sake of simplicity that the molecule was circular, this would correspond to a circumference of about 3.8 nanometres. For comparison: The largest machine operated at DESY is the PETRA III storage ring with a circumference of 2.3 kilometres – some 600 billion times larger.

# X-ray combination technique helps tuberculosis and osteoporosis research

Combination measurement shows distribution of metals in biological samples

Using an advanced X-ray combination technique, scientists have traced nanocarriers for tuberculosis drugs within cells with very high precision. The method combines two sophisticated X-ray scanning measurements and can locate minute amounts of various metals in biological samples at very high resolution. To illustrate its versatility, the researchers have also used the combination method to map the calcium content in human bone, an analysis that can benefit osteoporosis research.

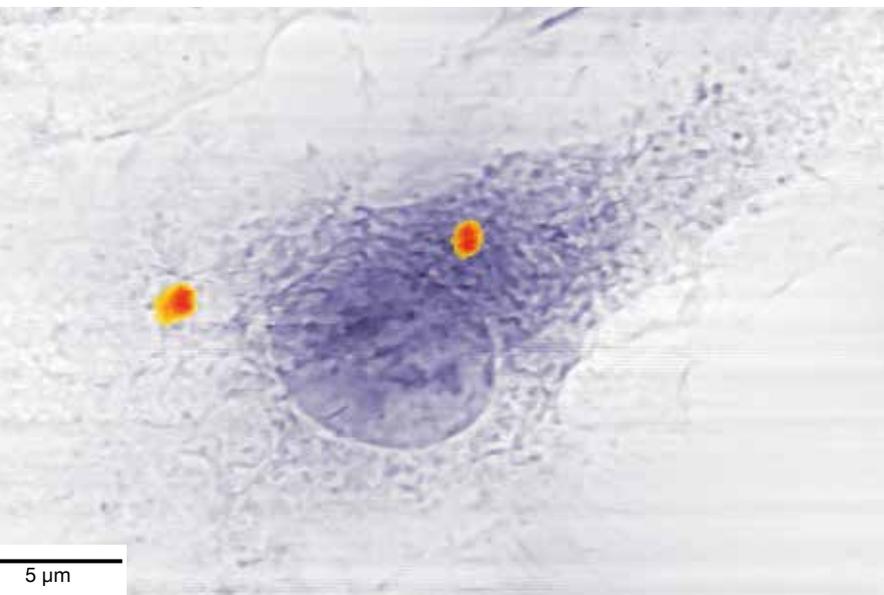
“Metals play key roles in numerous biological processes, from the oxygen transport in our red blood cells and the mineralisation of bones to the detrimental accumulation of

metals in nerve cells as seen in diseases like Alzheimer’s,” explains Karolina Stachnik, who works in the Center for Free-Electron Laser Science (CFEL) at DESY. High-energy X-rays make metals light up in fluorescence, a method that is very sensitive even to tiny amounts of metal. “However, the X-ray fluorescence measurements usually do not show the ultrastructure of a cell, for example,” says DESY scientist Alke Meents, who led the research. “If you want to exactly locate the metals within your sample, you have to combine the measurements with an imaging technique.” The ultrastructure comprises the fine details of the cell morphology that are not visible under an optical microscope.

## X-ray panorama image

As biological samples such as cells are very sensitive to X-ray radiation, it is highly beneficial to image their structure simultaneously to the fluorescence analysis in order to minimise radiation damage. For this reason, the team combined the fluorescence measurements with an imaging method known as ptychography. “A ptychographic microscope is fairly similar to taking a panorama image,” explains Stachnik. “An extended sample like a biological cell is raster scanned with a small coherent X-ray beam that produces many overlapping images of parts of the sample. These overlapping images are then stitched together afterwards.”

However, the X-rays do not directly produce pictures, but generate so-called X-ray diffraction patterns that are recorded on a detector. Each of these patterns contains information on the spatial structure of the respective part of the sample, which can be calculated from the pattern. “This finally results in a full quantitative optical density map of



Two agglomerates of antibiotic-loaded iron nanocontainers (red) in a macrophage

the sample,” explains Stachnik. “Through this complex process, ptychography provides spatial resolutions beyond the usual limits of X-ray optics.”

### Fluorescence maps

Thanks to its scanning nature, ptychography can be combined with the simultaneous acquisition of X-ray fluorescence measurements, which provide a unique fingerprint of the chemical elements in the sample. In this way, a picture of the sample’s morphology obtained by ptychography can be overlaid with an element map. “The concurrent combination of these two complementary imaging methods

“If you want to exactly locate the metals within your sample, you have to combine the measurements with an imaging technique“

Alke Meents, DESY

therefore enables artefact-free correlations of trace elements with the highly resolved sample structure,” summarises Meents.

A fundamental prerequisite for this method is that the X-rays are of a single colour only (monochromatic, all having the same wavelength) and that they oscillate in step (coherent) like in a laser. “Sufficiently bright, coherent, monochromatic X-rays with energies high enough to let metals like iron fluoresce have only become available at modern synchrotron light sources like DESY’s PETRA III,” says Meents.

To test the method, the DESY researchers teamed up with the group of Ulrich Schaible from the Research Center Borstel to investigate the localisation and concentration of nano-carriers for tuberculosis drugs within macrophages, the scavenger cells of the immune system. “Usually, macrophages



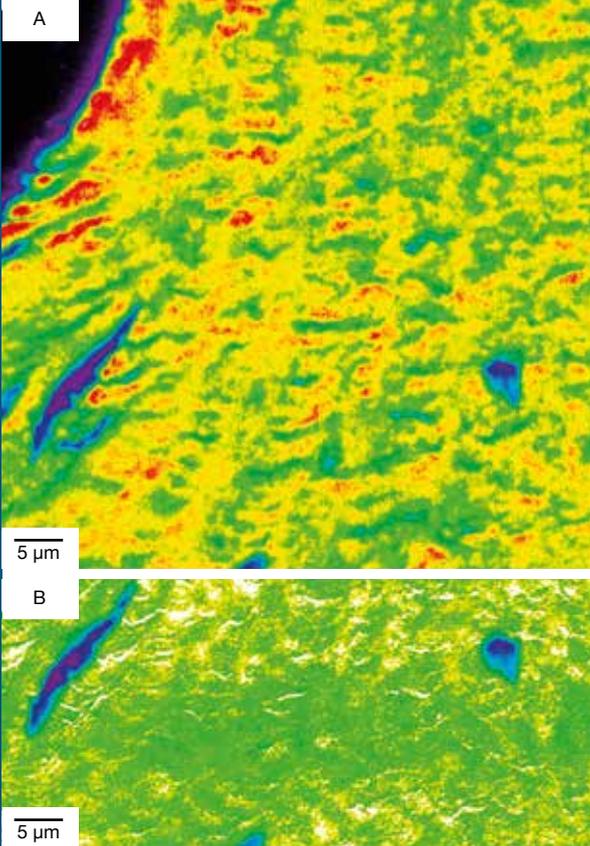
The tuberculosis pathogens *Mycobacterium tuberculosis* are rod-shaped bacteria. This computer-generated picture is based on images taken with a scanning electron microscope.

destroy pathogens like viruses and bacteria. Unfortunately, tuberculosis bacteria have managed to evade destruction and hide inside the macrophages instead, even using them to grow,” says Schaible. “One barrier for effective treatment is that the bacteria’s niches within the macrophages must first be reached by the antibiotics to be effective.”

### Nanocages made of iron

A new “Trojan Horse” strategy uses nanometre-sized iron containers to deliver antibiotics directly into the cells. These containers are hollow, filled with antibiotics and measure less than 20 nanometres in diameter (a nanometre is a millionth of a millimetre). “Macrophages swallow the containers, and once they are inside the cell, the iron walls of the cages slowly dissolve due to the need of the bacteria for iron. Eventually, the antibiotics are released and kill the bacteria,” explains Schaible.

To evaluate the efficacy of this strategy, the team investigated macrophages that had been fed iron containers. Using a specially >>



Calcium distribution in a human bone sample (top) and its mass-thickness-corrected section (bottom)

developed scanning stage at the bio-imaging and diffraction beamline of DESY's X-ray source PETRA III, the researchers could capture ptychographic and fluorescence images of 14 cells with subcellular resolution and identify a total of 22 agglomerates of nanocontainers within them.

### Calcium content in bones

In a second application, the researchers teamed up with the group of Björn Busse from the University Medical Center Hamburg-Eppendorf (UKE) and analysed the calcium content in a sample of human bone. "Calcium is a key element that makes our bones strong," explains co-author Katharina Jähn from Busse's group. "However, in times of high calcium requirement, the body dissolves it from the bones to use it elsewhere. These and other age-related processes can lead to osteoporosis, affecting nearly a quarter of all women at ages over 50 years in Germany."

Experimental research on bone mineralisation is usually performed on small slices of bone. "However, only the total content of calcium is usually mapped in this way," says Stachnik. "To get a true measure of the calcium concentration, one has to correct for the often varying thickness of the sample." The team used a simultaneously obtained ptychographic image to remove the mass-thickness distortion

from the calcium distribution map. "With this approach, we were able to observe a locally lower calcium content at certain points in the bone, which helps to better understand the process of bone disorders and to quantify the effect of bone mineralisation changes in patients," emphasises Stachnik.

### 3D measurements planned

To improve the method even further, the researchers have started to extend the analysis to three-dimensional measurements. "The experimental setup is currently being extended to allow the acquisition of 3D tomographic data sets," says Meents. "With many synchrotrons being upgraded to produce even brighter X-rays, we expect that this will significantly increase the sample throughput and make the method a routine application at these facilities."

*Scientific Reports, 2020; DOI: 10.1038/s41598-020-58318-7*

**"With this approach, we were able to observe a locally lower calcium content at certain points in the bone, which helps to better understand the process of bone disorders"**

Karolina Stachnik, DESY

# Spraying nanopaper

## Producing thin cellulose layers on an industrial scale

**W**ith a new spray coating process, very uniform layers of cellulose nanofibres (CNF) can be produced on an industrial scale. X-ray studies at DESY's research light source PETRA III as well as investigations with an atomic force microscope and using neutron scattering show how the layer is structured and can be tailored for different purposes, such as extremely thin, smooth and tough nanopaper.

### Renewable raw materials

"Porous, nanostructured cellulose films have a number of advantageous properties that make them interesting for various applications, from ultrastrong bioactive fibres to transparent conductive nanopaper," explains the main author of the study, Calvin Brett from DESY and the Royal Institute of Technology (KTH) in Stockholm. "They are lightweight and temperature-stable, have excellent mechanical properties and a low density and are made from renewable raw materials – cellulose nanofibres are usually made from wood."

This makes cellulose films a promising alternative to mineral-oil-based plastics and prospective candidates for the construction of functional materials such as bio-composites or biologically inspired sensors. For example, functional polymers or other substances can

The result is an extremely uniform, only 200 nanometre thick cellulose layer – a kind of ultrathin and extremely smooth paper. "A key question for the right properties is the relationship between the layering of the individual nanofibres, the porosity and

*"We have scaled up the process to such an extent that it is now possible for the first time to apply a cellulose film with a roughness of only two nanometres to a 50-meter-long foil"*

Calvin Brett, DESY and KTH Stockholm

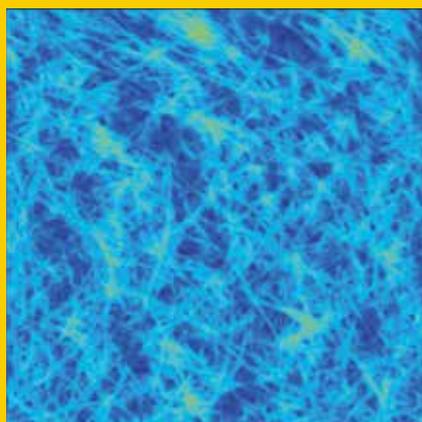
be introduced into the pores of the cellulose films in order to produce certain functions.

In the process developed at KTH Stockholm and DESY, cellulose nanofibres with an average length of 500 nanometres (millionths of a millimetre) and a typical thickness of 3 to 5 nanometres are sprayed onto a silicon substrate in a water-containing carrier liquid. The substrate is heated to 120 degrees Celsius in order to evaporate most of the water quickly and thus stabilise the cellulose layer.

the nanostructure within the cellulose film," explains DESY scientist Stephan Roth, who is also a professor at KTH Stockholm. "With our data, we can now tailor cellulose films for specific applications, for example with the optimum ratio between roughness, water content and voids."

### Industrial scale

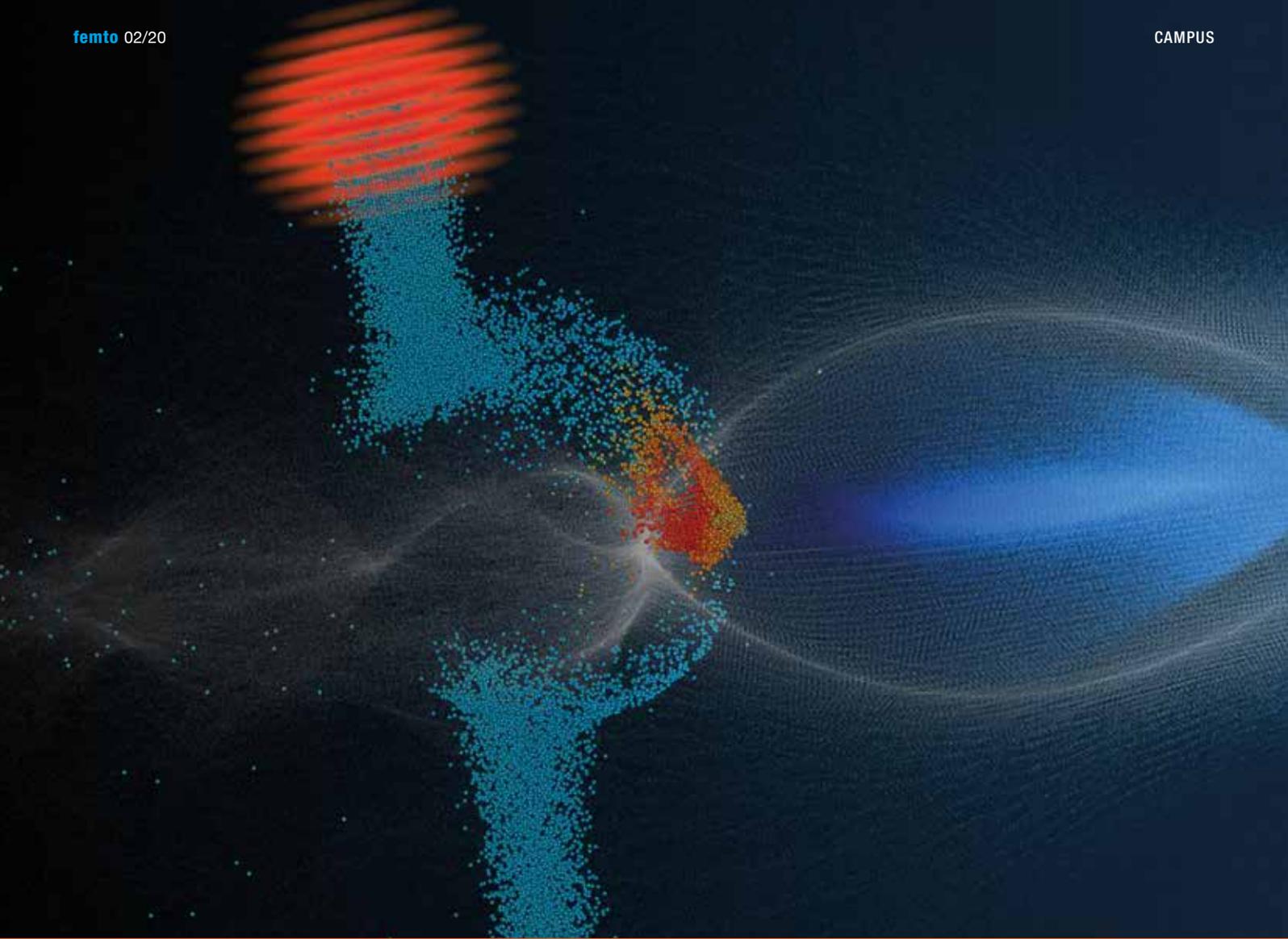
Such coatings can now be produced not only on a laboratory, but also on an industrial scale, emphasises Brett: "We have scaled up the process to such an extent that it is now possible for the first time to apply a cellulose film with a roughness of only two nanometres to a 50-meter-long foil." In the next step, the researchers plan to incorporate functional polymers into the cellulose film in order to produce a sensor material, for instance.



Measurements with an atomic force microscope show the nanopaper to be extremely smooth, varying only nanometres in height.

*Macromolecules*, 2019;

DOI: 10.1021/acs.macromol.9b0053



# “Trojan Horse” trick

## for ultrabrilliant electron beams

### Plasma photocathode for particle accelerators

**U**sing a trick modelled on the Trojan Horse, a novel electron source can generate extremely brilliant particle beams. The new method uses plasma acceleration technology and promises 100 to 10 000 times more tightly focused electron beams than conventional accelerators can currently deliver. An international team headed by Bernhard Hidding from the University of Strathclyde in

Glasgow, Scotland, has successfully tested the method at the SLAC National Accelerator Laboratory in California. DESY researchers played a major role in the work.

#### Versatile tools

High-energy electron beams are versatile tools for exploring the realm of molecules, atoms and elementary particles. They can either be used to collide electrons and their antiparticles,

positrons, in order to unravel the secrets of the subatomic world. Or they can be fed into specialised magnet arrangements to generate extremely bright X-rays, which can serve, for example, to observe proteins at work and to analyse the inner structure of new nanomaterials. “In any case, the colder and smaller the electron beams are, the better,” explains DESY physicist Alexander Knetsch, co-author of the publication.

Illustration, based on simulations, of the Trojan Horse technique: A laser beam (red) strips electrons (light blue dots) off of helium atoms. Some of the freed electrons (red dots) get accelerated inside the plasma bubble (white elliptical shape) created by another, high-energy electron beam (dark blue).

ride like a surfer on an ocean wave. This plasma wakefield can accelerate particles much more strongly over short distances than the best conventional accelerators available today. However, plasma wakefield acceleration is still in the experimental phase, and there are only few applications yet.

#### Precisely targeted laser pulses

“The colder the electrons are at the beginning of the acceleration, the slower they move relative to one another, and the closer they stay together – an important prerequisite for strongly focused beams,” says Knetsch. For their method, the physicists released cold electrons into the hot plasma bubble in a similar way to how the Greeks allegedly once smuggled soldiers into the besieged city of Troy in a wooden horse. Instead of a wooden horse, however, helium atoms served as hiding places for the electrons.

The researchers used a mixture of hydrogen and helium gas. The laser that generated the plasma was just energetic enough to release the electrons from the hydrogen atoms, but not from the helium atoms. The scientists thus produced a plasma wave from the hydrogen gas, while the helium remained unimpressed. With a precisely targeted second laser pulse, which had a slightly higher energy, they then released electrons from their “Trojan Horses”, the helium atoms, right inside the plasma bubble. These still cold electrons were generated in a tiny region of a few thousandths of a millimetre in diameter and even more strongly compressed by the directly following plasma wave.

“Our experiment shows for the first time that the ‘Trojan horse’ method actually works,” emphasises Hidding. “It’s one of the most promising methods for future electron sources and could push the boundaries of today’s technology.” The plasma setup takes over the

function of the photocathode, which is commonly used as an electron source for conventional particle accelerators. In these highly specialised devices, a laser knocks electrons out of a piece of metal, captures them with a strong electromagnetic field and bundles and packs them into bunches that are finally fed into the accelerator.

The electrons from the plasma photocathode that has now been successfully tested could also be

*“It’s one of the most promising methods for future electron sources and could push the boundaries of today’s technology”*

Bernhard Hidding, University of Strathclyde

fed into a particle accelerator, but they can also be accelerated to high energies directly in the plasma itself. In the pilot experiment, the electrons reached up to 700 mega-electronvolts. The researchers estimate that the beam quality can already compete with the one delivered by conventional electron sources. In further experiments, the scientists will now aim to increase the quality and stability of the beam and also to improve the beam diagnostics.

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The team tested a process in which “cold” electrons with just little kinetic energy are accelerated by a plasma wave. A plasma is a gas in which the electrons have been stripped from the molecules or atoms so that the gas has two electrically oppositely charged components. If a strong laser pulse or a high-energy electron bunch is fired into the plasma, it generates an electrically charged wave in its wake on which electrons can



## “Beamline for Schools” at DESY

“DESY Chain” and “Particle Peers” – these are the names of the two teams of young scientists, from Salt Lake City in the USA and Groningen in the Netherlands, who won the international “Beamline for Schools” competition in 2019. They spent two weeks carrying out experiments at the particle accelerator DESY II in Hamburg.

“Beamline for Schools” (BL4S) is a competition in which teams of young people from all over the world come up with experiments that can be carried out using a particle beam. In 2019, 178 teams from 49 countries submitted proposals. Usually, the winners of BL4S are invited to CERN in Geneva, Switzerland. However, all the accelerators at CERN are currently shut down while the Large Hadron Collider (LHC) is being upgraded, so the teams are coming to DESY instead. The next round of experiments is to take place this autumn. Despite the coronavirus pandemic, even more applications were received this year than last. The winners are to be announced this summer.

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