femto

The DESY research magazine – Issue 01/22

ENGLISH EDITION

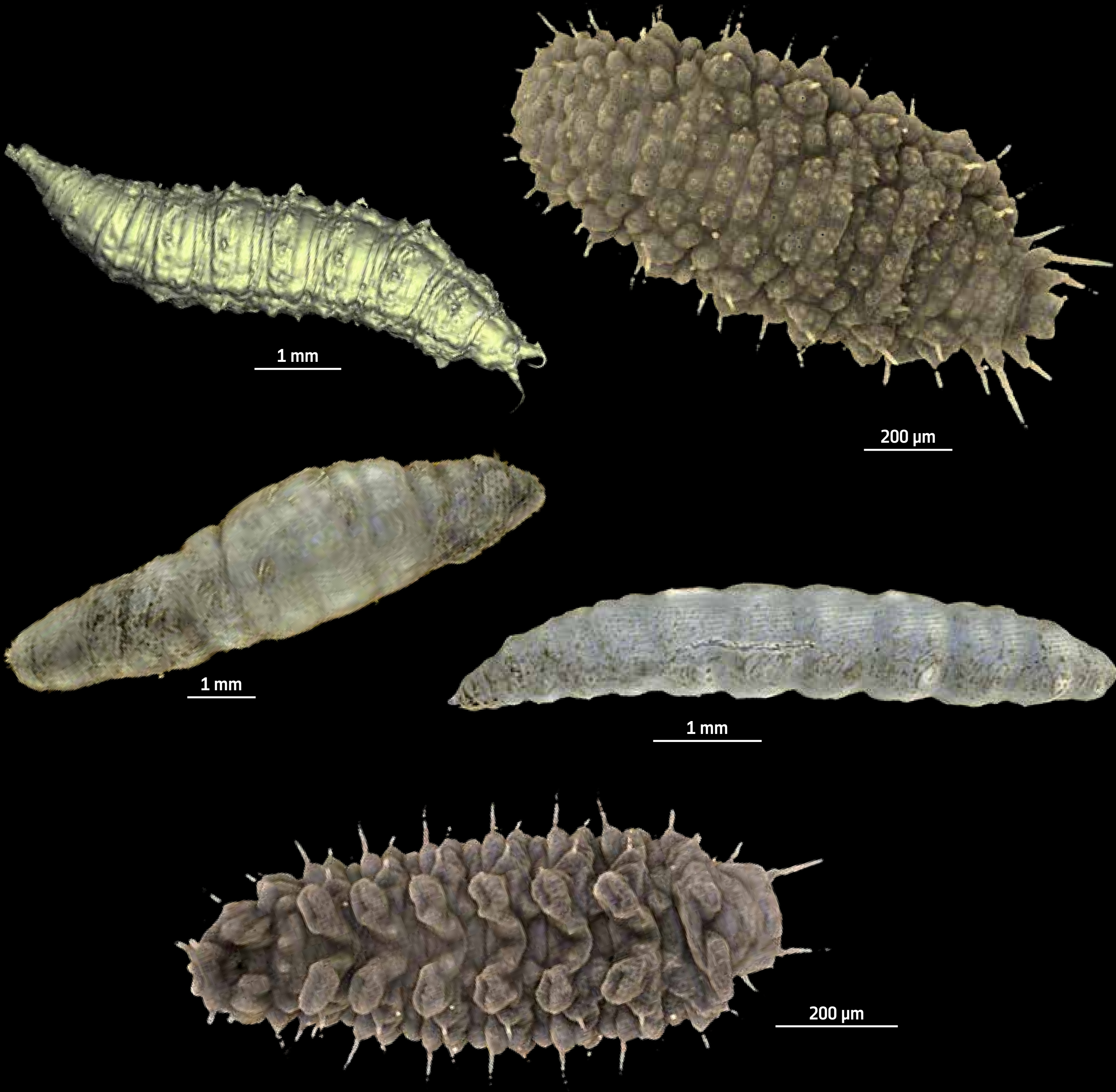
THE SECOND QUANTUM REVOLUTION

Cosmic chemistry in the lab

Coronavirus damages heart vessels

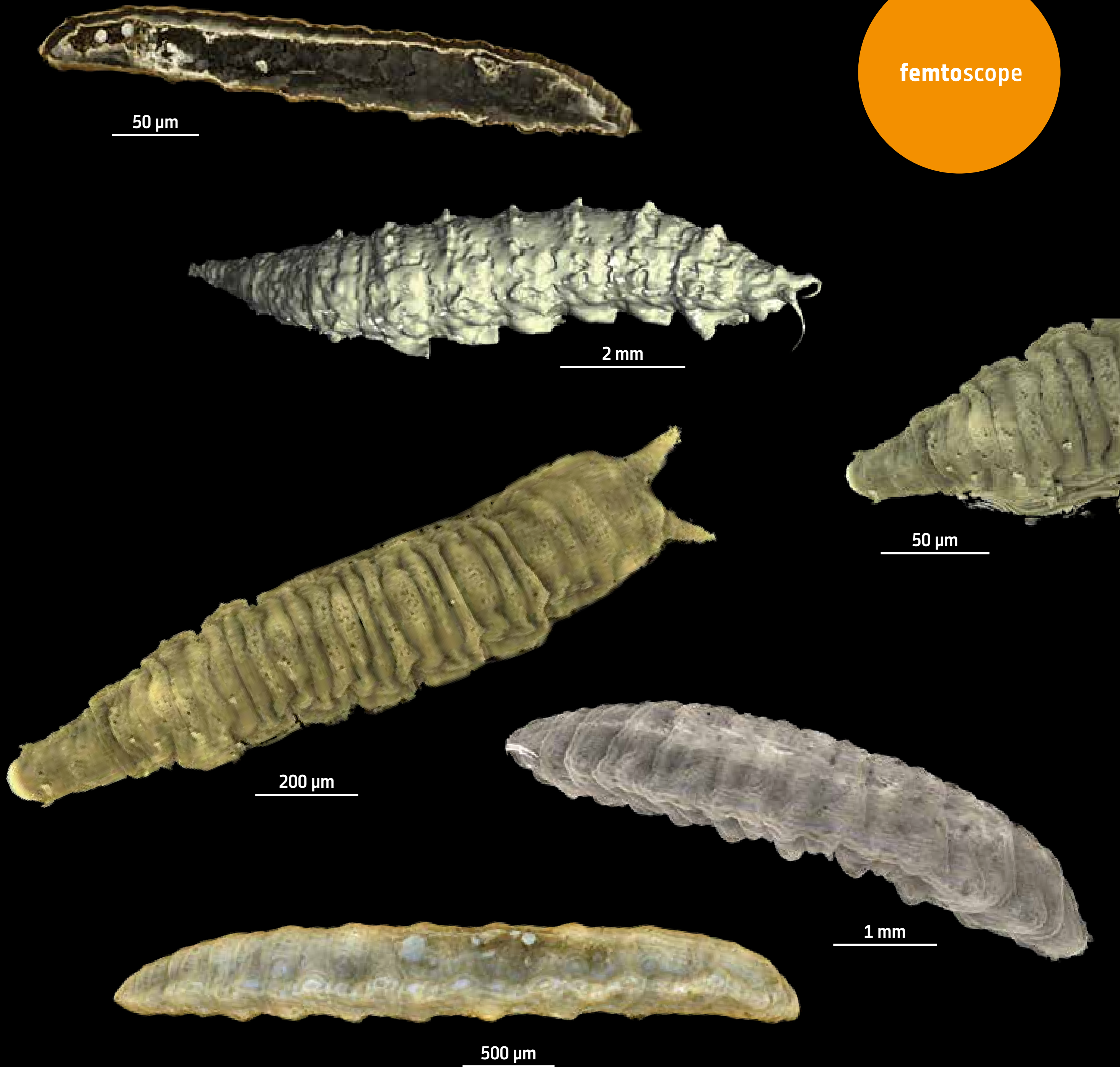
Radiolarians as a design model

DESY.



Scanning the past

In the late Eocene period – around 38 to 34 million years ago – the Baltic amber forests covered large areas of what is now Northern Europe. The resin of these forests is the source of most amber found in Europe. In one sample, researchers led by Viktor Baranov and Joachim Haug from Ludwig-Maximilians-Universität in Munich have discovered a surprising variety of fly larvae – a total of 56 fly larvae, all of which were entombed while feasting on a single chunk of mammalian dung. "This fossil is particularly interesting because the dung is full of plant residues, which implies the presence of at least moderately large herbivores in these forests," Baranov explains. On this basis, he and his colleagues assume that there must have been open areas of femtoscope



Pictures: Viktor A. Baranov, Michael S. Engel, Jörg Hammel, Marie K. Hörnig, Thomas van de Kamp, Marcus Zuber and Joachim T. Haug; „Palaeontologia Electronica", 2021; DOI: 10.26879/1129

grassland nearby, corroborating earlier hypotheses. "The Baltic amber forest is often portrayed as a densely overgrown and humid jungle landscape. But it is much more likely that it was a more open, warm-to-temperate habitat," Baranov says.

Great diversity

Using the bright and intense X-ray light from DESY's synchrotron radiation source PETRA III, the scientists examined the larvae in detail and were able to take extremely detailed pictures of the ancient fossils. "The imaging basically works in the same way as with a computer tomograph, only with micrometre resolution," explains co-author Jörg Hammel from Helmholtz-Zentrum Hereon. Hereon operates the experimental station at PETRA III where the images were taken. A micrometre is one thousandth of a millimetre.

In total, the researchers were able to identify 20 different so-called morphotypes of larvae, including 11 new ones that were only described in this study. "The great diversity of larvae on the faeces suggests that fly larvae already played an important role in recycling organic matter in the amber forest," the scientists explain in the journal "Palaeontologia Electronica", in which they report on their work.

Palaeontologia Electronica, DOI: 10.26879/1129

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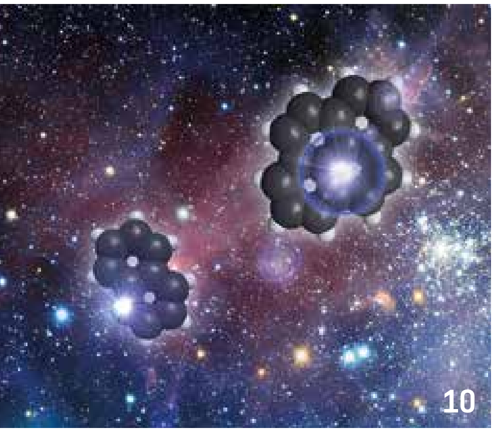

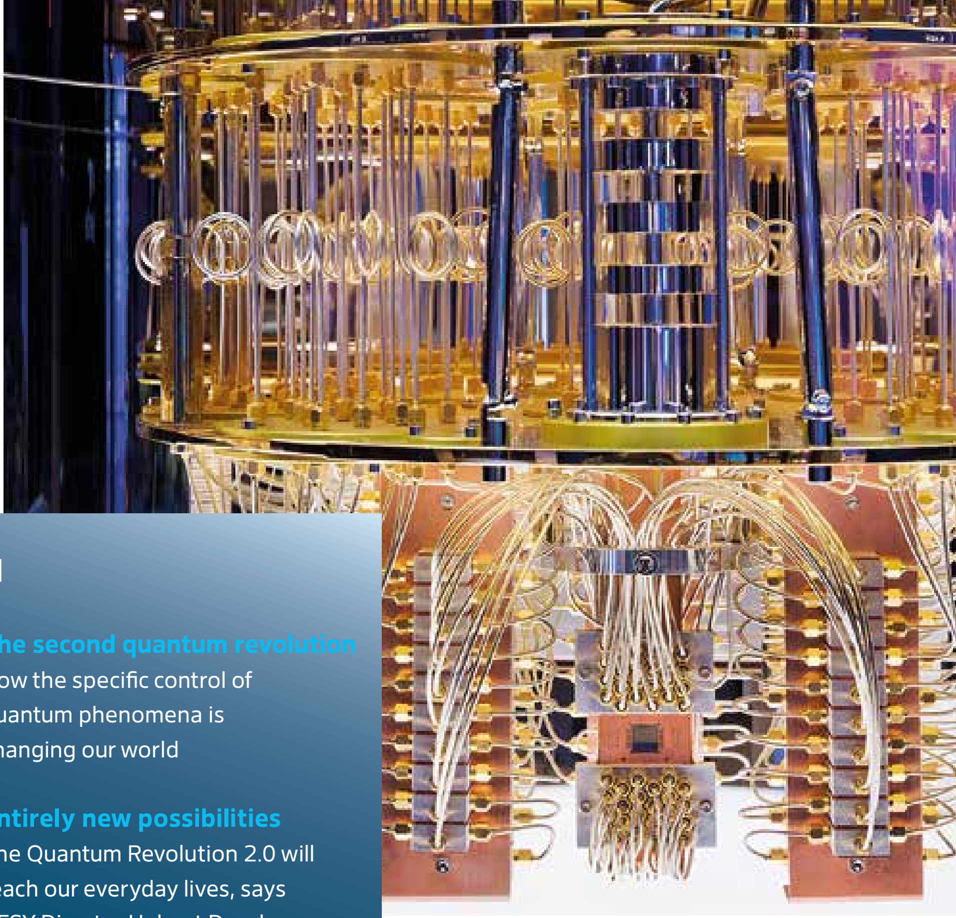

ZOOM


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Dear Readers,

How often have you used quantum technologies today? Glancing at your smartphone, the laser scanner at the supermarket checkout, the microwave oven in your kitchen – quantum technologies are all around us. In the past 120 years or so, quantum physics has revolutionised the way we view the world, but also our everyday lives. And along the way, it has created a market that is worth billions.

First-generation quantum technologies, such as transistors and lasers, specifically exploit certain quantum phenomena. We are now witnessing the beginning of a second quantum revolution: Having understood quantum phenomena, researchers are learning to control them.

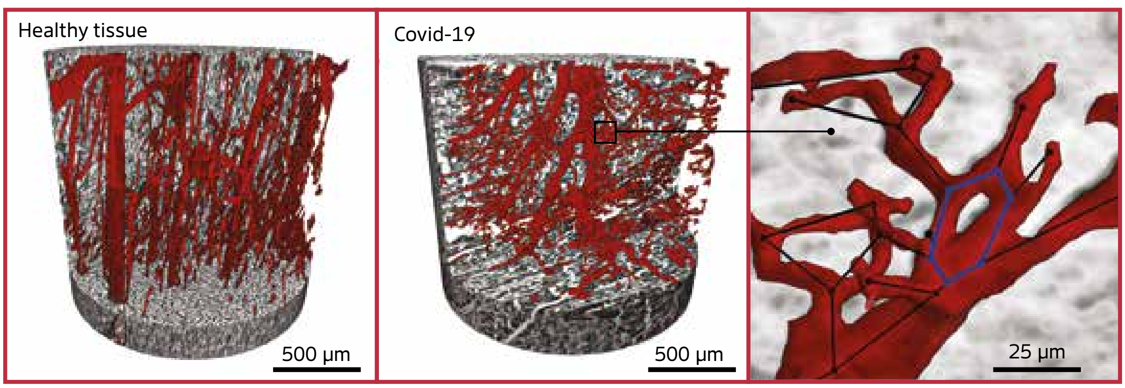
Expectations towards the resulting second-generation quantum technologies are high: Quantum computers are supposed to handle hitherto intractable big-data analyses, but also carry out AI simulations, financial market analyses and traffic control tasks. Quantum communication is to make the Internet faster, data safer and navigation much more accurate. And quantum sensors are to shrink large, expensive devices, such as magnetoencephalographs, down to a convenient size so that they can be brought directly to patients, for example.

In this issue, you will read about how researchers are juggling quanta, which applications of Quantum Technology 2.0 are already being explored and what challenges still lie ahead. We hope you enjoy reading it and find it enlightening, and we look forward to hearing any criticism, praise or suggestions you would like to share with us at femto@desy.de.

Till Mundzeck
Editor

Covid-19 can cause vascular damage to the heart

Innovative X-ray imaging provides first direct proof



Vascular network (red) in healthy heart tissue (left) and in severe Covid-19 (right). Due to faulty reforming of the network as a result of Covid-19, numerous branches, splits and even loops develop in the capillaries, which can be analysed mathematically using graphs.

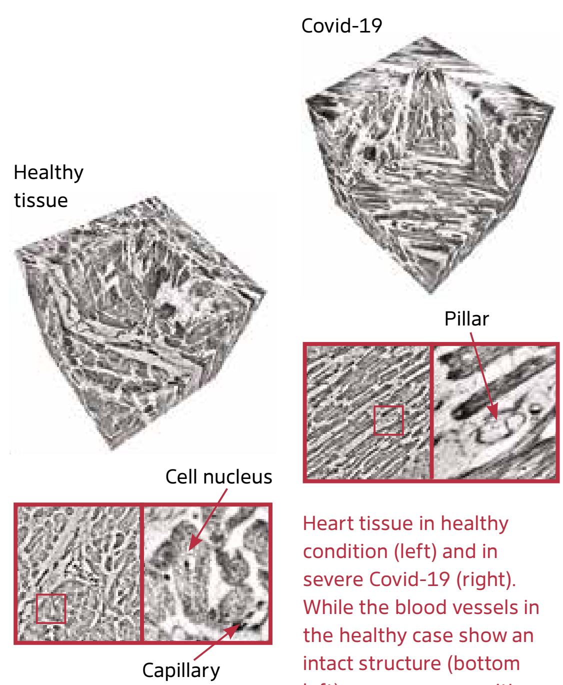
The coronavirus not only attacks the lungs, but can also damage the vessels in the heart. Using DESY's X-ray light source PETRA III, an interdisciplinary research team led by the University of Göttingen and Hannover Medical School (MHH) has detected significant changes in the heart muscle tissue of people who died from Covid-19. The study underpins the involvement of the heart in Covid-19 for the first time at the cellular level by imaging and analysing the affected tissue in three dimensions.

For their study, the scientists imaged the tissue architecture at high resolution using the particularly bright X-rays of PETRA III and displayed it in three dimensions. To do this, they used a special X-ray microscope set up and operated at DESY by the University of Göttingen. In the severe disease courses of Covid-19 studied, the researchers observed clear changes at the level of the tiny blood vessels, the capillaries, in the heart muscle tissue.

Chaotically rebuilt network

In comparison with a healthy heart, the X-ray images of tissues affected by severe disease revealed a network full of splits, branches and loops that had been chaotically remodelled by the formation and splitting of new vessels. These images are the first direct visual evidence of a special form of new vessel formation in the tissue called "intussusceptive angiogenesis", which is one of the main drivers of the known and already well-studied lung damage in Covid-19. In order to visualise the capillary network, the vessels in the three-dimensional volume first had to be identified using machine learning methods. This initially required the researchers to painstakingly label the image data.

"To speed up image processing, we therefore also automatically broke the tissue architecture



Heart tissue in healthy condition (left) and in severe Covid-19 (right). While the blood vessels in the healthy case show an intact structure (bottom left), one can see cavities or pouches and tiny pillars forming in the fine blood vessels (capillaries) in the Covid-19 tissue sample, which indicate particular morphological changes.

Pictures: University of Göttingen, M. Reichardt/P. Møller Jensen/T. Salditt; University of Göttingen, M. Reichardt/T. Salditt down into its local symmetrical features and compared them," explains Marius Reichardt from the University of Göttingen, the first author of the paper. The parameters obtained showed a completely different quality compared to healthy tissue or even to diseases such as severe influenza or common myocarditis, as the leaders of the study, Tim Salditt from the University of Göttingen and Danny Jonigk from MHH, report.

The study has a very special feature: In contrast to the vascular architecture, the data quality required here could be achieved using a small X-ray source in the laboratory of the University of Göttingen. In principle, this means that this could also be done in any clinic to support pathologists with routine diagnostics. In the future, the researchers want to further expand the approach of converting the characteristic tissue patterns into abstract mathematical graphs

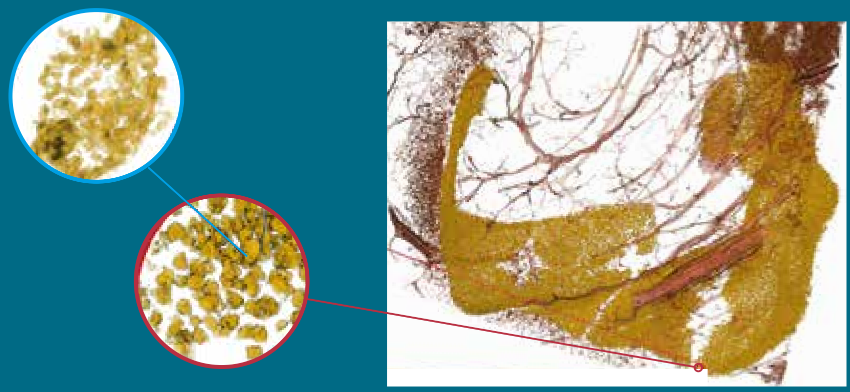
"We automatically broke the tissue architecture down into its local symmetrical features and compared them"

Marius Reichardt, University of Göttingen

in order to create automated tools for diagnostics, again by further developing laboratory X-ray imaging and validating it with synchrotron radiation from PETRA III. To this end, the collaboration with DESY will be further expanded in the coming years.

eLife, DOI: 10.7554/eLife.71359

UNPRECEDENTED INSIGHTS INTO THE BRAIN OF ALZHEIMER'S PATIENTS



Neuronal cell nuclei of the so-called *dentus gyratus* (yellow) and associated blood vessels (red). By varying the magnification of the X-ray optics, one can zoom in on the densely packed band of neurons (in the red oval) and also resolve the substructure of the cell nucleus (blue oval, around 0.015 millimetres in diameter).

Picture: University of Göttingen, M. Eckermann/T. Salditt

Innovative X-ray imaging can not only detect vascular damage caused by Covid-19, it also offers new insights into the brain tissue of Alzheimer's patients. Researchers at the University of Göttingen and the University Medical Center Göttingen took a new approach to analyse the neuronal tissue architecture in three dimensions and at high resolution using DESY's X-ray source PETRA III. The team was able to detect a previously unknown transition in neuronal cell nuclei in tissue samples from Alzheimer's patients, which indicates an altered activity of the neurons.

The scientists examined neuronal tissue from the hippocampus, a brain region where memories are transferred from short-term to long-term memory. The researchers used a special phase-contrast tomograph, which the team led by Tim Salditt had set up at PETRA III. The tomograph can be used to image tissue that absorbs X-rays only weakly or even not at all. This meant that large volumes of tissue could be recorded in their entirety, without damaging the samples and without time-consuming preparation.

"To do this, the three-dimensional image from highly magnified projections must first be focused on the computer using special algorithms in order to obtain a three-dimensional image with pixel sizes in the range of one ten-thousandth of a millimetre," explains the first author of the paper, Marina Eckermann from Göttingen. With this "digital twin" of the sample, machine learning can then be used to identify neurons – excitable cells that send information between different areas of the brain by means of electrical impulses and chemical signals. Using new mathematical methods developed by Bernhard Schmitzer at the University of Göttingen, the team compared samples from different individuals.

"These new results show that, in Alzheimer's disease, the cell nuclei in a subsection in the hippocampus change into being more compact and having more of a mixture of different structures," explains Salditt. "This leads to a higher proportion of densely packed DNA in the cell nucleus and to DNA being read out less frequently," says Christine Stadelmann-Nessler from the University Medical Center Göttingen. "Whether the observed changes in the cell nucleus also play a causal role in the development of the disease remains to be seen."

Proceedings of the National Academy of Sciences (PNAS), DOI: 10.1073/pnas.2113835118

The 4.5-metre-high large volume press weighs in at 35 tonnes and can exert a pressure of 500 tonnes on each of its three axes, corresponding to 300 000 times the atmospheric pressure or the pressure conditions 900 kilometres below Earth's surface. During compression, the samples' inner structure can be analysed using the bright X-ray light from PETRA III.

High-pressure view into the Earth

Mineral transformation causes puzzling change in speed of earthquake waves

At a depth of 660 kilometres below the Earth's surface, earthquake waves abruptly change their speed. This so-called seismic discontinuity is one of the most striking structural boundaries in the Earth's mantle. However, for reasons as yet unknown, this structural boundary splits into two discontinuities in some places: Where oceanic crust dips below continental crust, discontinuities lie in the range of 660 to 670 kilometres and 740 to 750 kilometres deep.

Using high-pressure experiments, a research team led by the University of Bayreuth has now recreated the conditions in the sinking Earth plates while illuminating the samples at DESY's X-ray light source PETRA III and the Japanese X-ray source SPring-8. The investigation provides an explanation for the puzzling phenomenon: According to the study, the splitting of the structural boundary is caused by the transformation of a special mineral.

Such a transformation is also responsible for the usual seismic discontinuity in the transition zone from the upper to the lower mantle at a depth of about 660 kilometres: There, ringwoodite, which is composed of magnesium, iron, silicon and oxygen, breaks down into the minerals bridgmanite and ferropericlase. As a result, seismic waves can propagate faster.

The splitting of this structural boundary into two separate discontinuities is only seen below so-called cold subduction zones – areas of sinking Earth plates where temperatures are still searingly high, but much cooler than in normal subduction zones. The dissociation of ringwoodite cannot be responsible for the splitting of the structural boundary under these zones, however, as it is largely independent of the temperature and therefore always occurs under the pressure that prevails at a depth of around 660 kilometres.

Plausible explanation

The researchers, led by first author Artem Chanyshev from DESY and the University of Bayreuth, have therefore studied the behaviour of another mineral: Akimotoite occurs mainly in the cooler areas of the transition zone to the lower mantle and also transforms into bridgmanite. "We loaded mineral samples into our large volume press and analysed them with the bright X-rays from PETRA III while compressing and heating them," explains co-author Robert Farla, scientist in charge of the beamline at DESY where the experiments took place. "In this way, we can follow structural changes in the minerals under conditions of the Earth's mantle."

The experiments show an unexpectedly strong temperature dependence of the phase transition from akimotoite to bridgmanite: The lower the temperature, the higher the compression pressure must be for the phase transition to happen. However, higher pressure is only reached at a greater depth. Even a comparatively small drop in temperature therefore causes the phase transition from akimotoite to bridgmanite to shift significantly deeper into the Earth's interior. "On the basis of our experiments, the very striking seismic discontinuity at a depth of 740 to 750 kilometres below cold subduction zones can be plausibly explained by the akimotoite–bridgmanite phase transition," reports Chanyshev.

Nature, DOI: 10.1038/s41586-021-04157-z

Pictures: DESY, Franziska Lorenz & Jochen Stuhrmann (illustrato); DESY, Marta Mayer

"There are still many questions"

Beate Heinemann is a professor of physics and DESY's new Director in charge of Particle Physics since the beginning of 2022. DESY's first female director wants to encourage young women researchers and looks forward to possible revolutionary discoveries in the future.

femto: In the more than 60 years that DESY is existing now, you are the first woman on the Board of Directors. Why has it taken such a long time?

Beate Heinemann: Well, it's the same in many other organisations; it has taken them 50 years or longer, and there are still a great many that have never had a woman in a top management position at all. Unfortunately, we are still a long way from having truly equal opportunities for women and men in society, but at least things are moving forward, though a little slower than I would like. When I did my PhD here at DESY, there were far fewer outstanding women in all areas of public life, including science. I very much hope that the next woman will join DESY's Board of Directors quite soon, not in another 60 years!

femto: Do you see yourself as a role model for other women researchers?

Beate Heinemann: I think that's inevitable. When you are one of a relatively small number of women in a highly visible position, you are de facto a role model, whether you like it or not. Looking back, all the women I met in research were basically role models for me. And few things would make me happier than for my being here to contribute in some way to encouraging young women researchers to get involved and to voice their opinions.

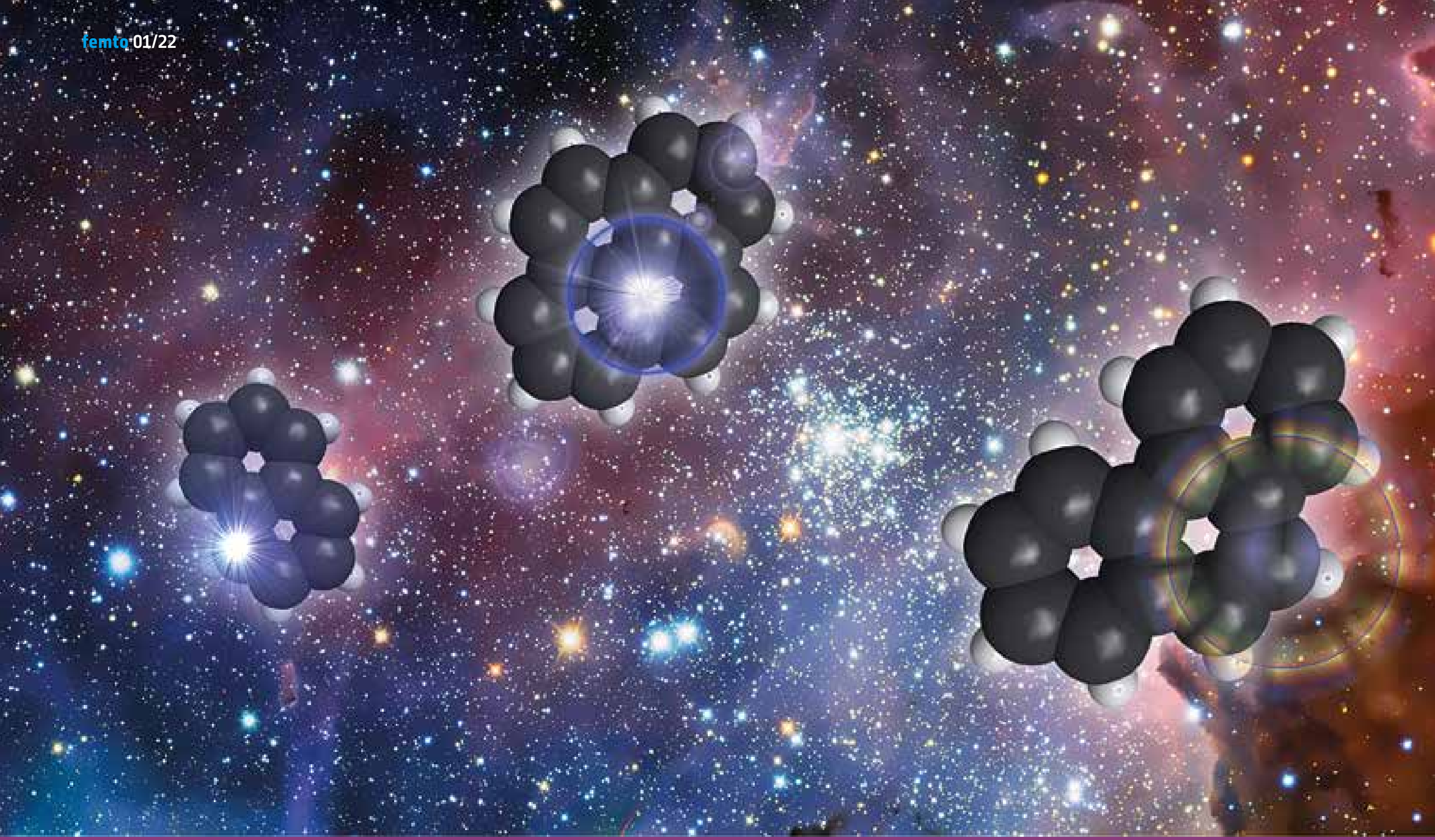
femto: You are Director in charge of Particle Physics. What are the key questions for particle physics in the next few years?

Beate Heinemann: The largest and most important project in particle physics continues to be the Large Hadron Collider at CERN. At DESY, we are heavily involved in the analyses, but also in the operation of the ATLAS and CMS detectors, as well as in software development and computing. In principle, the LHC can provide answers to many fundamental questions, such as the nature of dark matter, the structure of the vacuum, why there are different types of matter, and more beyond. But the perhaps most exciting discoveries right now are in the field known as B physics, where recent measurements indicate that two different types of elementary particles, electrons and muons, behave somewhat differently from what was expected. If these indications are correct, other new particles or forces must be involved. Our work on the Belle II experiment in Japan is also very important here. The search for dark matter is not confined to the LHC either. At DESY, we have an axion programme, which is really taking off right now with the ALPS II experiment. Axions are hypothetical light elementary particles that could make up dark matter. We intend to add further axion experiments at a later date. And then we are planning LUXE, an experiment to study quantum physics in extremely strong electromagnetic fields. Werner Heisenberg dreamed of doing this back in the 1930s, but it has only recently become technically feasible.

femto: Ten years ago, the Higgs boson was discovered. What might be the next great breakthrough in particle physics?

Beate Heinemann: That's highly speculative, of course! There are still a great many questions and incongruities, and the range of energies that we are able to achieve at the LHC, for example, will presumably provide the key to some of the answers. It's very exciting to be advancing into regions that no human being has ever explored before. This has often led to revolutionary discoveries in the past, and I'm convinced that this will continue in the future too.

Picture: DESY, Angela Pfeiffer



Cosmic chemistry in the lab

Research team simulates the harsh environment of interstellar space

Carbon compounds play a special role in our world: The entire chemistry of life is based on these so-called organic molecules. In the universe, much of the carbon is contained in a group of simple compounds called polycyclic aromatic hydrocarbons (PAHs). Using DESY's free-electron laser FLASH, scientists have now recreated some of the harsh environment of interstellar space in the lab and analysed the reaction of these astrochemically important molecules to these conditions.

The results advance our understanding of organic chemistry in space, emphasises the international team led by Bastian Manschwetus and Melanie Schnell from DESY. Organic chemistry deals with the reactions, composition and properties of molecules containing carbon (C). PAHs are an important group of fundamental organic compounds, consisting of carbon and hydrogen (H). The results show a comprehensive picture of the dynamics of polycyclic aromatic hydrocarbons under extreme ultraviolet radiation in a vacuum – resembling the cosmic environment between the stars of our galaxy.

Less than a trillionth of a second

"Polycyclic aromatic hydrocarbons are found in almost every corner of the universe, accounting for up to 20 percent of all carbon in space," explains Jason Lee from DESY, one of the paper's main authors. "These molecules play an important role in interstellar chemistry, providing reaction surfaces, aggregating into larger species such as fullerenes and fragmenting into building blocks for other organic molecules, among other things. Our work aims at understanding the reaction dynamics of PAHs following interaction with the ionising radiation found in interstellar space."

The scientists investigated the response of the three small PAHs fluorene ($C_{13}H_{10}$), phenanthrene ($C_{14}H_{10}$) and pyrene ($C_{16}H_{10}$) to the extreme ultraviolet (XUV) radiation from FLASH. The XUV flashes were tuned to a wavelength of 30.3 nanometres, matching an important emission line of helium in interstellar space. For comparison: Visible light has wavelengths between 400 and 800 nanometres.

Picture: DESY, Bastian Manschwetus (background: NASA/Hubble)

Polycyclic aromatic hydrocarbons (PAHs) are compounds consisting of carbon rings (black) with various numbers of hydrogen atoms (grey) attached. Infrared observations show that these molecules are ubiquitous in space.

The extreme ultraviolet photons can knock up to three electrons out of a PAH molecule, leading to a highly ionised state. With a specialised instrument, the CAMP measuring station, and a superfast camera, called PImMS, the team was able to disentangle the complex fragmentation and ionisation dynamics of the molecules. The analysis shows that all investigated PAHs respond extremely quickly following the absorption of the high-energy radiation, redistributing the energy into atomic movement in much less than a picosecond (trillionth of a second). State-of-the-art theoretical calculations had already predicted roughly the same time scale for this process, which is known as relaxation.

“PAHs are found in almost every corner of the universe”

Jason Lee, DESY

Doubly charged

The data reveal details of the reactions of the PAHs to the intense radiation: If, for example, two electrons are kicked out of a PAH molecule by an XUV photon, a doubly electrically positively charged ion is formed. According to the experiments, such dications preferentially split into two fragments, each of which carries a single electric charge and is therefore called a monocation. This splitting into two monocations is often accompanied by the loss of two carbon atoms (C_2). This is especially intriguing for astrochemists, as it mirrors the proposed mechanism for creating PAHs in the first place. According to this common conception, the various PAH molecules build up gradually as acetylene molecules (C_2H_2) join together sequentially.

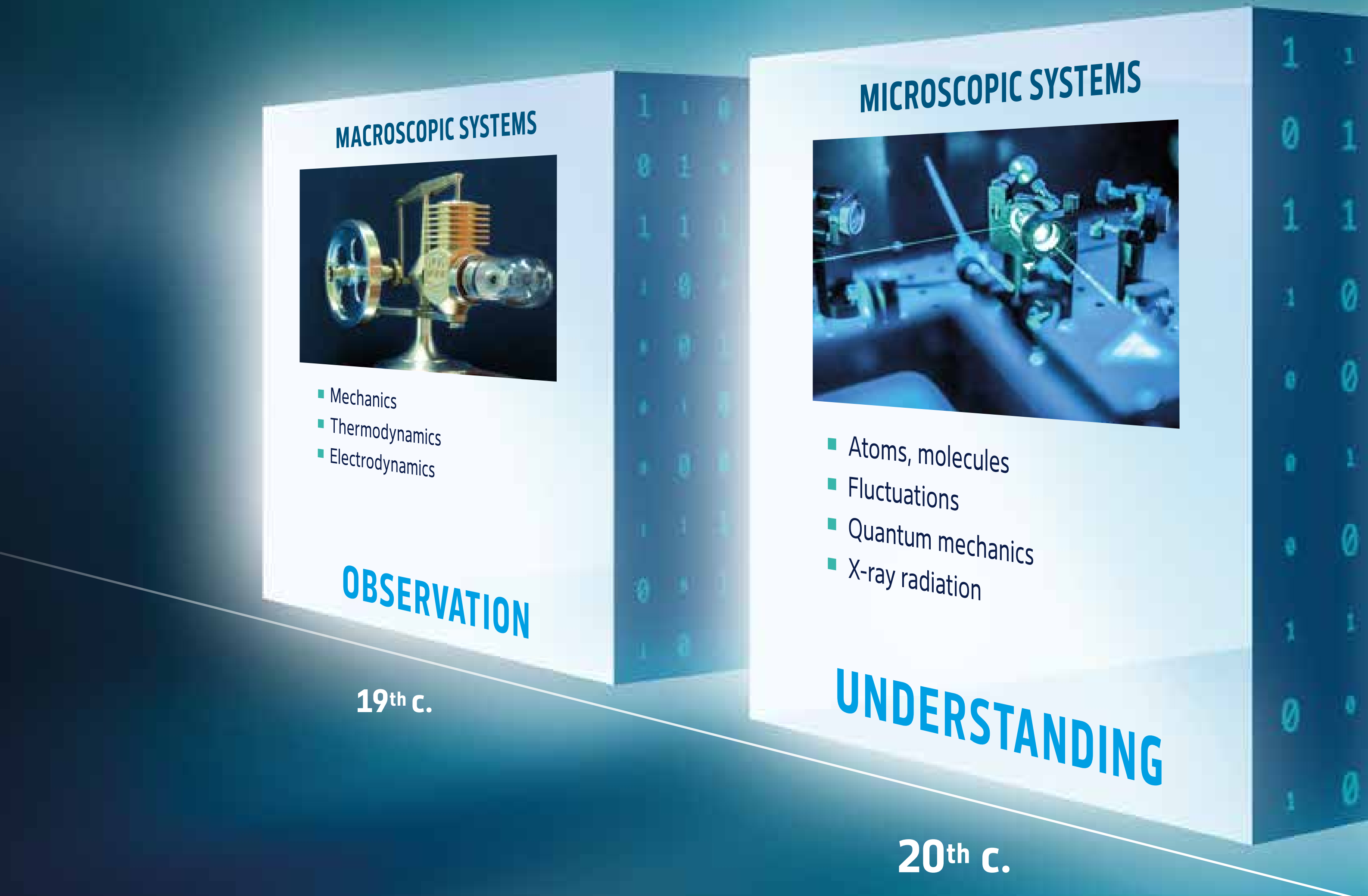
“Our results show that ultrafast relaxation may be ubiquitous amongst polycyclic aromatic hydrocarbons,” says Lee. The team is already evaluating further experiments at FLASH with a new group of PAHs to confirm this observation. The analysis of the fragmentation of triply charged PAH molecules (trications) is so elaborate that the team will report on it in a follow-up article.

The work, which involved an international team of scientists from the universities of Oxford, Kiel, Lund, Gothenburg, Hamburg, Amsterdam, Göttingen, Radboud University in Nijmegen, Saint Petersburg State University, Kansas State University, Vrije Universiteit Amsterdam, the European XFEL X-ray laser and DESY, provides valuable insights into the interaction of this group of organic molecules, which are widespread in the cosmos, with interstellar radiation. The ions and fragments that are created in the process provide the building blocks for more complex molecules and thus decisively shape the organic chemistry of the cosmos.

Nature Communications,
DOI: 10.1038/s41467-021-26193-z

The experimental setup in the laser tent with the ultrafast camera PImMS at the CAMP measuring station (monitored by the mascot Clyde, above)

Pictures: Maciej Tomiczek (portrait); DESY, Jason Lee

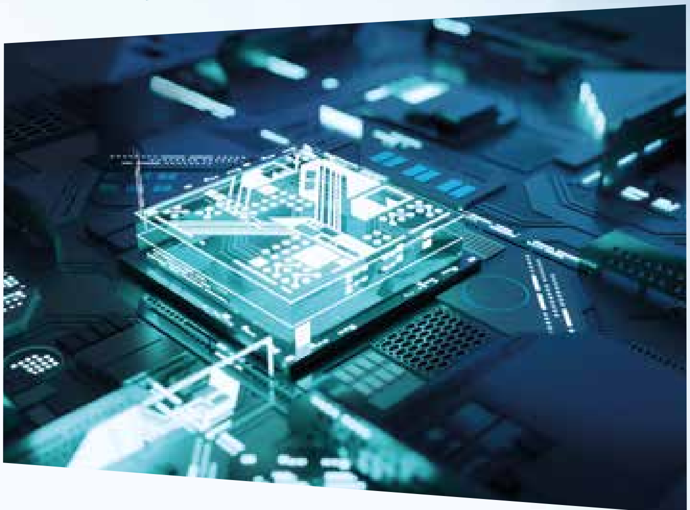


THE SECOND QUANTUM REVOLUTION

Quantum physics has revolutionised the world – changing our understanding of nature and our everyday lives. With the first quantum revolution, a few decades ago, quantum technologies such as transistors and lasers became commonplace. These are the fruits of an ever deeper understanding of the laws of quantum physics. However, most of the practical applications of quantum phenomena were not even imaginable when these were first discovered. Today, the world is on the brink of a second quantum revolution. In the meantime, it has become possible to identify, control and manipulate

Graphic: Carolin Rankin, DESY

QUANTUM SYSTEMS



- Control of quanta in matter and energy
- Quantum technologies
- Multifunctional materials
- Medical active ingredients
- Digital twins

CONTROL

Today

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ZOOM

individual quantum objects such as photons, electrons, atoms and molecules so reliably that entirely new techniques are now possible: quantum sensors that allow measurements to be made with unprecedented precision. Or quantum materials that could form the basis of future electronic devices. Or quantum computers that can operate at far higher speeds than today's computers. For science, the second quantum revolution holds the promise of new tools for gathering knowledge, while industry anticipates new markets worth billions.

Pictures: fdecomite, CC BY 2.0 / istockphoto, Михаил Руденко / istockphoto.com, solarseven

The airport staff is stretched to the limit: The weather has gone haywire, most flights are delayed, countless passengers risk missing their connections. To keep the chaos in check, every flight that arrives ideally needs to be directed to a specific gate so as to minimise transfer times. This may sound simple – but in mathematical terms, the problem of finding the best gate for such a large number of planes in a matter of minutes is a Herculean task that even supercomputers often fail to solve today.

In the future, it could be mastered by an entirely new type of computer, one based on the arcane rules of quantum physics: a quantum computer. These computers are part of an emerging field of research known as quantum technology. All over the world, countless laboratories in industry and science are working on quantum computers. Not only optimisation tasks such as airport routing ought to be child's play for such computers; they will also be able to conduct fast searches in databases, complex calculations and elaborate computer simulations and to run artificial intelligence (AI) algorithms. What makes quantum computers so special is that they operate according to a completely different principle from conventional processors. The latter do their calculations using bits, i.e. units of memory that are either zero or one. Quantum computers, by contrast, are based on qubits (quantum bits), which can take on arbitrary combinations of one and zero at the same time and therefore represent an infinite number of values.

Karl Jansen is a co-coordinator for quantum technologies at DESY and head of the Centre for Quantum Technology Applications (CQTA).

More information than atoms in the universe

Connecting up several quantum bits results in a very powerful computer. Whereas a ten-bit PC can encode one of about a thousand possible values, one after the other, the quantum computer is able to take on all those thousand different values at once in ten qubits. A system with one thousand qubits could in principle store more information than there are atoms in the universe. As a result, such a computer ought to be able to perform certain operations much more quickly, making it more climate-friendly and sustainable than today's supercomputers – provided it is suitably programmed using the right algorithm.

This means that quantum computers could be helpful, for example, when searching certain databases or as an AI tool for detecting anomalies, such as suspicious tissue structures in an X-ray image. They should also be able to solve optimisation problems in the field of logistics, for example: How does a parcel service find the shortest route for delivering its shipments? A highly complex system, characterised by a maze of streets in a city, but also by road works and traffic jams. Today, logistics companies already rely on high-performance computers to optimise their transport routes. The expectation is that quantum algorithms could identify significantly faster and better solutions by exploiting quantum-mechanical principles. Moreover, quantum computers seem predestined for running computer simulations. This is because they are suitable for simulating quantum systems, i.e. the behaviour of molecules and materials – and not just their state at a particular point in time. This could be useful when designing specific drugs, for example, or materials, such as for better batteries.

"This is the right time to develop algorithms so as to make the best use of quantum computers once the time comes"

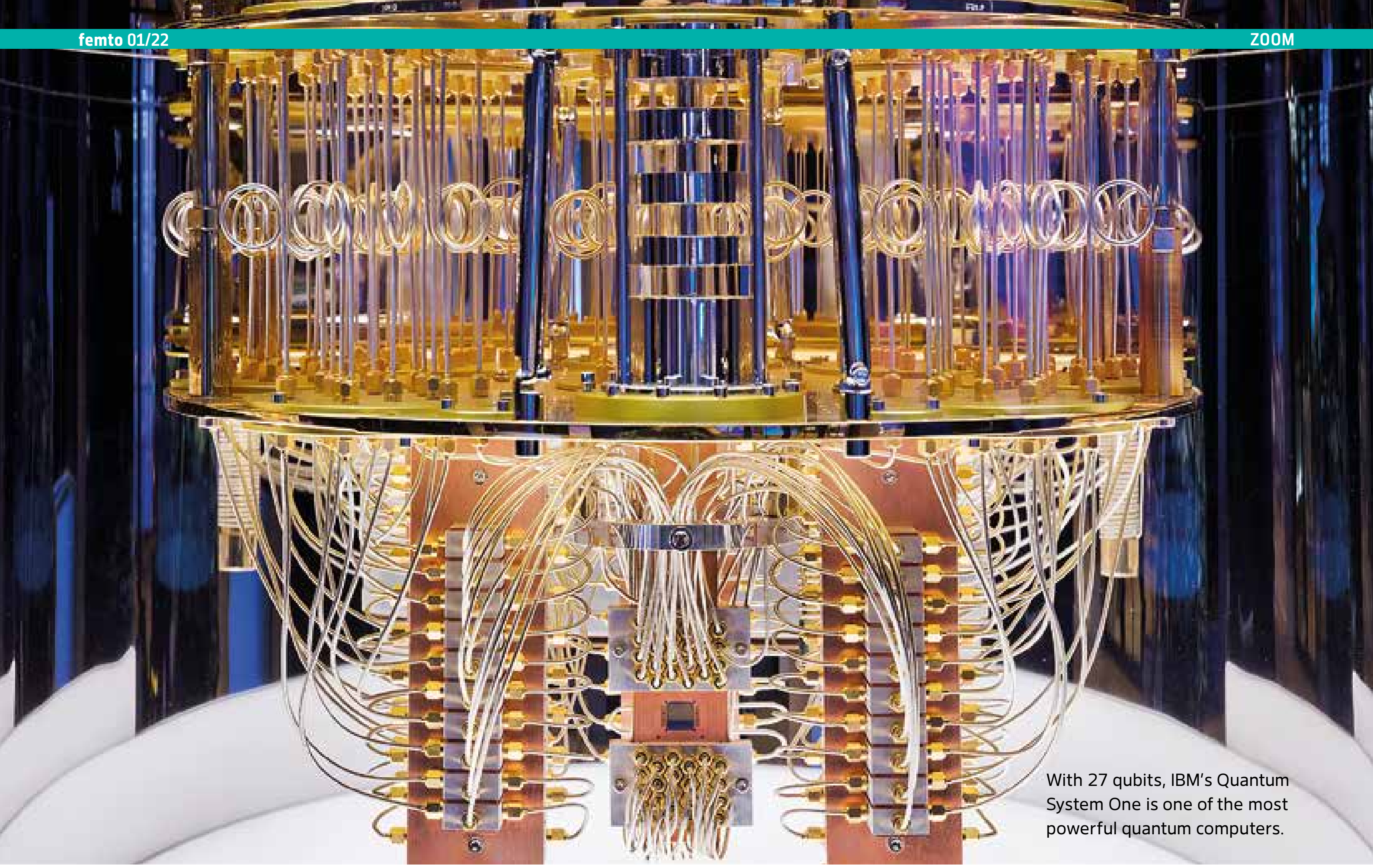
Karl Jansen, DESY

One million qubits

Until now, though, this technology has only led to a limited number of practical applications. This is because today's prototypes of a universal quantum computer only have a few dozen qubits – too few to keep up with ordinary computers. And "at the moment, quantum computers are still very sensitive to noise. Even the slightest interaction with the environment can seriously disrupt them," according to DESY physicist Karl Jansen, who is the head of the Centre for Quantum Technology Applications (CQTA). "So a large number of errors still occur during the calculations."

But development is making progress: Companies such as IBM and Google have announced that they will be launching systems with a few hundred or thousand qubits over the next few years, and by 2030 this could even reach a million. Recipes also exist against the susceptibility to error: One method employs dozens or even hundreds

Picture: DESY, Gesine Born



With 27 qubits, IBM's Quantum System One is one of the most powerful quantum computers.

of additional qubits for each qubit to check and correct the results calculated by the first one. Other approaches try to correct the errors using artificial intelligence or neural networks.

It will probably still be a while before fully functional quantum computers are available. But the possibilities they could then offer are not even conceivable today. "When the laser was developed, no one thought that one day people would use it to perform eye surgery," says Peter Zoller, Director of the Institute of Quantum Optics and Quantum Information at the Austrian Academy of Sciences. "Perhaps, in the future, quantum computers will also open up realms that we are not even dreaming of today."

Promising prospects

The experts also have high hopes for quantum sensors. These can be made from specially prepared diamonds, for example, and are to detect brain waves, magnetic forces or gravitational fields much more precisely than has hitherto been possible. A new generation of atomic clocks could optimise satellite navigation – every GPS satellite has an atomic clock on board. More accurate clocks might allow navigation systems to determine the position of a car to within a centimetre – something that is important for autonomous driving, for example.

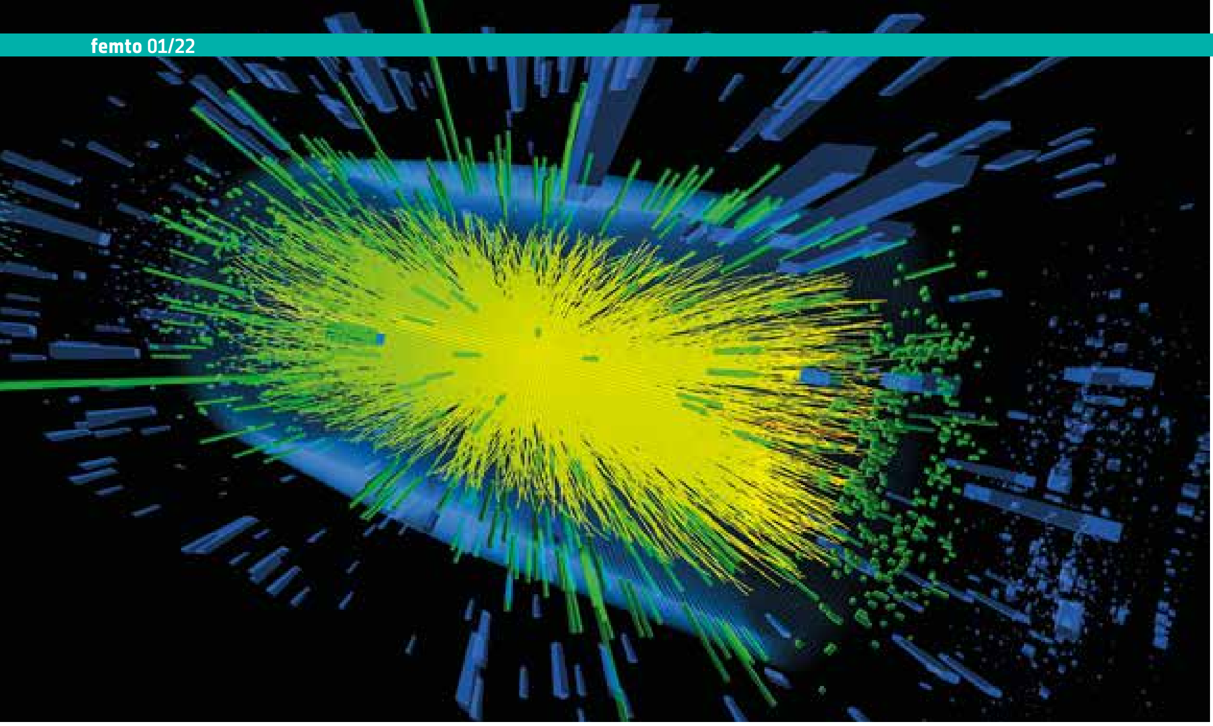
Quantum materials also offer promising prospects. In them, electrons interact in unusual ways with each other and with the crystal lattice. This leads to special electronic properties that could, among other things, make faster and more efficient computer chips possible, but also superconductors that carry electric current without any losses, not only at extremely low temperatures but even at room temperature.

"All these technologies have huge potential for the future," says Kerstin Borras, who coordinates quantum technology at DESY together with Jansen. Like the qubits in a quantum computer, research relies on synergies: Progress can be achieved more quickly when partner institutions collaborate. It is not just business and industry that stand to profit

> *"Perhaps quantum computers will open up realms that we are not even dreaming of today"*
>
> ***Peter Zoller, Austrian Academy of Sciences***

from quantum technologies in the future, but also science. Quantum computers could, for example, help scientists analyse the highly complex data collected in particle accelerator experiments or tackle theoretical problems that are very difficult or impossible to solve ››

Picture: IBM



The particle collisions in the Large Hadron Collider generate huge quantities of data, which will increase significantly in the future. Quantum computers could help analyse them.

today. Quantum sensors could keep a lookout for previously undiscovered elementary particles. And using DESY's X-ray sources, promising quantum materials can be studied in extreme detail and optimised for special applications, such as a quantum computer with low error rates.

Flood of data from particle collisions

"A quantum computer would be interesting, for example, in connection with the experiments at the particle physics research centre CERN in Geneva and specifically at the LHC, the largest particle accelerator in the world," says Kerstin Borras, who is involved in CMS, one of the large detectors at the LHC. The underlying principle is that the 27-kilometre ring accelerator drives protons (hydrogen nuclei) to extremely high energies and then makes them collide head-on. In these collisions, elementary interactions lead to the creation of countless particles, which fly apart in different directions.

Huge detectors such as CMS observe what happens and record the signals produced by the particles, which are very fast and very tiny, as precisely as possible. By analysing the measured data, it is then possible to determine whether new, previously undiscovered particles were created during the collisions or whether deviations from the theoretical predictions indicate that new physics was involved. This is how the famous Higgs boson was tracked down at the LHC in 2012 – a discovery for which the theoretical physicists Peter Higgs and François Englert were awarded the Nobel Prize in 2013.

Every collision in the LHC produces a large number of particles that have to be taken into account. This is why analysing the LHC data has until now only been possible with massive and novel computing assistance: The World Wide Web was invented at CERN for the worldwide exchange of data, and the global computer grid was also developed at the time when the LHC came into being. "Over the coming years, these analyses are going to become even more challenging," Borras reports. "The LHC is currently being upgraded so that, in a few years' time, it will be able to fire many more protons at each other than it does now, generating a much larger flood of data."

Kerstin Borras is a lead scientist and co-coordinator for quantum technologies at DESY and a professor at RWTH Aachen University.

"These technologies have huge potential for the future"

Kerstin Borras, DESY

Big-data challenge

The plan is for up to 200 interactions to take place simultaneously, which will produce enormously dense particle signals. "The new conditions are a major big-data challenge. To my mind, quantum computers offer a great opportunity here," says Borras. In order to explore the potential of the new technology, Borras took the initiative and set up a quantum technology task force, ››

Pictures: CERN

“ENTIRELY NEW POSSIBILITIES”

Controlling specific quantum properties paves the way for innovative technologies

The discovery of quantum mechanics changed the basic laws of physics and laid the foundations for revolutionary new technologies. Now, DESY Director Helmut Dosch believes, the Quantum Revolution 2.0 will turn our everyday lives upside down once again.

femto: In the early 20th century, physicists discovered that the world is made up of quanta. Why was this a revolution?

Helmut Dosch: Before that, people had a very macroscopic view of matter – the formulae describing mechanics and electrodynamics were considered to be the basic laws of physics. But then the observational tools improved, and it became increasingly clear that matter is composed of atoms and molecules. These no longer obey the classical laws of physics, however; instead, they follow the new rules of quantum mechanics, which take some getting used to. Its laws state, among other things, that atoms can behave not only as particles but at the same time also as waves. This fundamental understanding later became the basis for technologies such as microchips and lasers, which shape our everyday lives today. That development is known as the first quantum revolution.

femto: We are now facing a second quantum revolution. What is its distinguishing feature?

Helmut Dosch: For technologies such as lasers and transistors, it was necessary to understand the quantum world. But science is now able to specifically control quantum properties – such as the spooky entanglement that can exist between two quantum systems. Today, this can be exploited to allow the qubits in a quantum computer to jointly perform calculations, which they can do much more quickly than an ordinary computer. This promises entirely new possibilities for the future.

femto: What has science already achieved? What challenges still lie ahead?

Helmut Dosch: In the case of quantum computers, there are prototypes that prove that the principle works. The aim here is now to build larger devices with significantly more qubits, which are also less susceptible to disruption. Some approaches already exist, but we may still have to develop completely new technologies, for example based on new types of quantum materials. Other quantum technologies, such as quantum cryptography, are already much further. This allows data communication using light quanta that is not susceptible to eavesdropping. Devices that can be used over short distances are already available for sale.

femto: How can research at DESY contribute to this?

Helmut Dosch: DESY can support this research in several respects. One example is that we are working on quantum algorithms for particle physics that will assist the analysis of data from accelerator experiments. We can run these algorithms on new quantum computer prototypes that are currently being developed in numerous laboratories. This allows us to test their performance and to carry out a form of benchmarking, which then helps us with their further development. Our X-ray sources PETRA III, FLASH and the European XFEL, in which DESY plays a major role, are equally important. Their high-intensity radiation allows novel quantum materials to be studied in extremely great detail. And such materials could then form the basis for future quantum computers and quantum sensors.

femto: Will we one day carry around quantum computers in our pockets?

Helmut Dosch: Quantum computers are likely to be used primarily in data centres. There, they could allow routes to be calculated more quickly, for example, but also help people to develop better drugs and materials. However, this technology is likely to be too complex for a PC or a smartphone in the foreseeable future. What is more readily conceivable, though, is that smartphones will one day be fitted with a quantum cryptography chip. This could ensure that data can be transmitted without being susceptible to eavesdropping, thereby providing risk-free Internet communications.

Picture: DESY, Rüdiger Nehmzow

RACE OF THE SYSTEMS

For now, it remains unclear which underlying principle future quantum computers will be based on. Some approaches are already quite advanced, allowing working prototypes to be built. Others are still in their infancy, but hold great promise for the future. Some examples:

SUPERCONDUCTING QUBITS: These are based on micrometre-small circuits made of a superconducting material, which are interrupted by tiny gaps, so-called Josephson junctions. When these are cooled down close to absolute zero, currents flow through them without any losses – either clockwise or anticlockwise. The directions of rotation can be superimposed with the help of microwaves to create a quantum bit. This is the principle used by IBM and Google, for example.

QUBITS FROM ION TRAPS: Individual ions are trapped in a vacuum chamber by magnetic fields. Short laser pulses put the electrons in the ions into different, specific states. During this process, two different states can be superimposed, creating a quantum bit. Several ions can be locked up in adjacent traps. They can interact with each other and together form a larger processing unit.

QUBITS FROM SEMICONDUCTORS: Here, the basis is formed by materials used to manufacture computer chips. Experts use a chip made of high-purity silicon, for example, into which they specifically insert an atom of phosphorus. The nucleus and one electron from this atom each act as a quantum bit. The chip manufacturer Intel is pursuing a similar approach.

QUBITS FROM DIAMOND DEFECTS: A diamond can be turned into a quantum bit by a sophisticated process: A carbon atom in its crystal lattice is replaced by a nitrogen atom, with a lattice vacancy right next to it. This tiny ensemble acts like an artificial molecule and a stable quantum bit, which can be manipulated using laser pulses and radio waves.

together with Karl Jansen and like-minded people from all of DESY's research divisions.

The scientist is already working on quantum algorithms to simulate and analyse the data collected in the particle physics experiments at CERN. Specifically, the self-learning software operates according to the principle of a neural network, a program architecture that is modelled on the way the human brain works. Although it is still under development, Kerstin Borras hopes that, by 2029, when the upgraded LHC is due to go into operation, the quantum algorithms will be so powerful as to contribute significantly to the particle hunt.

Other physical phenomena should also be much easier to model and simulate with the help of quanta – from superconductivity to the emerging class of materials known as topological insulators. "A quantum computer might also be interesting for simulating the early universe, when it was small and its density and temperature were extremely high," says Jansen. "That is scarcely possible using a classical computer."

Quantum technology centre

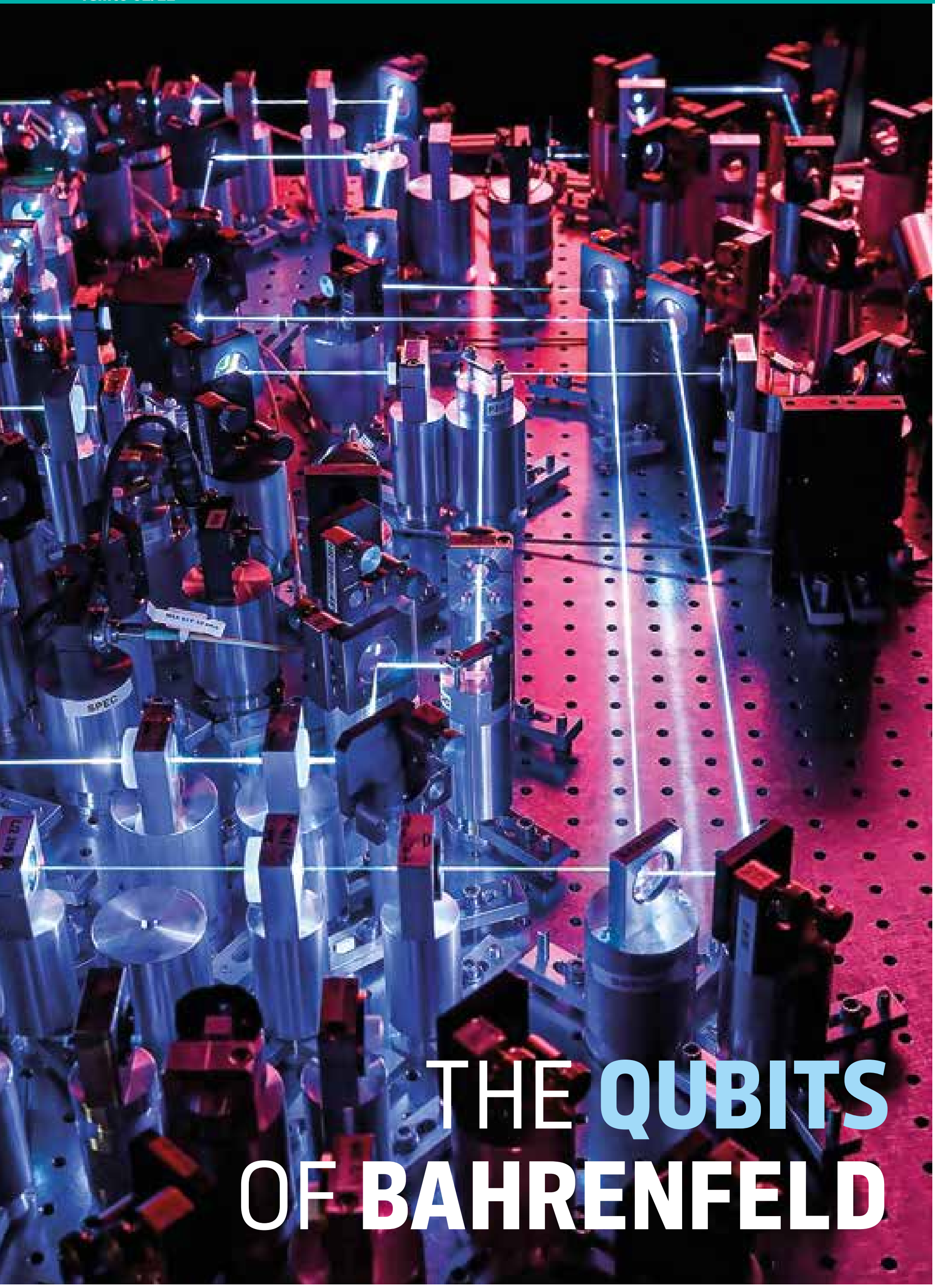
As recently as 2019, Jansen believed that quantum computing was a technology for the distant future. But then he became aware of the Californian start-up Rigetti Computing, a company that offers access via the Internet to a small quantum computer that has just a few qubits. Visiting their website, Jansen had a startling experience: "I was able to control the quantum computer from my own home, using my laptop and an ordinary programming language that I was already familiar with," he says. "That was a paradigm shift for me."

The physicist decided to delve deeper into this technology of the future and soon recognised its potential for research. In the end, he initiated a new centre at DESY's Zeuthen site, the Centre for Quantum Technology Applications (CQTA), to systematically explore the possibilities of quantum computers and to develop concrete applications for this new miracle in computing. The centre will receive a total of 15 million euros in funding from the Future Investment Fund of the German federal state of Brandenburg over a period of five years.

"Quantum ready"

"Our centre will offer experts at DESY and also many other users access to IBM's quantum computers," explains Karl Jansen. IBM is one of the leading manufacturers and offers its partners cloud access to the computational powers of its quantum computers. For the time being, the capacity of these devices is still limited. But the company is already holding out the prospect that, in a few years' time, quantum processors will be available that are – at least in certain respects – superior to today's supercomputers.

The technology is therefore approaching the threshold for practical applications. "This is the right time to develop algorithms so as to make the best use of quantum computers once the time comes," Jansen emphasises. "And we need to find out for which applications quantum computers will be particularly useful." This investigation at the new centre in Zeuthen will not be confined to DESY's own projects: "We want to approach other research institutes as well as companies and offer them our support," says Karl Jansen. "We would also like to be a go-to for smaller companies that just want to give quantum computing a try." Another important aspect of the new centre is in the field of education and training, he adds: "We want to offer tutorials and courses to familiarise people working in business and science with this new method of programming and thus get them 'quantum ready'."



The quantum computer Rymax One uses lasers to hold individual atoms and put them into so-called Rydberg states, which can adopt carefully controlled, highly entangled quantum states.

Picture: UHH-CUI, Peter Garten

THE QUBITS OF BAHRENFELD

The Institute for Laser Physics at Universität Hamburg is building a quantum computer based on suspended atoms

Lightning-fast database searches, comprehensive simulations, cracking unsolvable codes – all this could be child's play for a quantum computer. For a long time, only laboratory devices were available, offering a modest performance. But for some years now, their development has been gathering momentum. IT companies such as Google, IBM and Microsoft are investing millions and millions in research, while banks, logistics companies and automotive groups are sounding out the possibilities offered by the miraculous computers to come.

It remains to be seen, however, what the systems will look like in the future. Research groups around the world are currently working on very different technologies in order to build a truly powerful quantum computer: Some rely on superconducting quantum bits, others on trapped ions, others again on diamonds spiked with nitrogen. "At the moment, there's a race going on, and no one knows who will win it," says Klaus Sengstock from the Institute for Laser Physics at Universität Hamburg. "But everyone takes it for granted that powerful quantum computers will eventually arrive." Conceivably, different systems will specialise in different tasks.

Laser beams as tweezers

On the Hamburg-Bahrenfeld research campus, the team of Henning Moritz, Peter Schmelcher and Klaus Sengstock is working on a special version of the quantum computer in a project called Rymax. The principle behind it is that laser beams in a vacuum chamber act as tweezers, holding hundreds of ytterbium atoms suspended, arranged into a regular lattice in which the individual atoms are a few micrometres apart. A small amount of energy is then carefully pumped into the atoms, again by a laser. As a result, one of the electrons in the atomic shell is lifted into a remote "orbit". Figuratively speaking, this inflates the atom into a giant structure known as a Rydberg atom. By clever illumination with the laser beam, this Rydberg atom can be programmed as a qubit and made ›› to perform calculations. The result is read out by special cameras.

The advantage of this approach is that, due to their size, the Rydberg qubits can "talk" to each other over comparatively long distances, meaning that they can be joined up to form switching units that can perform calculations together. On top of this, the atoms can be moved by the laser tweezers as if by a tractor beam in order to perform computations with other qubits. "We can control, address and measure our quantum bits very precisely using laser beams," says Sengstock – a direct expression of the second quantum revolution.

Lorry-induced "quantum crash"

The roadmap is for the researchers to gradually add more and more qubits to their laboratory setup, until it reaches a total of 500. They hope to end up with a "quantum annealer" – a special type of quantum computer that specialises in

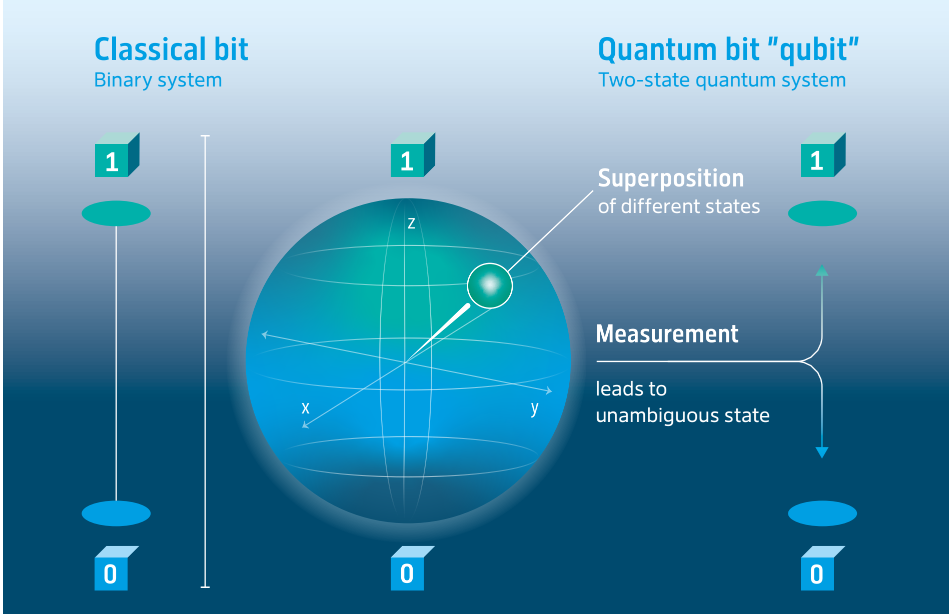
"At the moment, there's a race going on, and no one knows who will win it"

Klaus Sengstock, Universität Hamburg

solving optimisation problems. The underlying principle is that "we create an ensemble of qubits and program it such that it tries to minimise its energy," explains Sengstock. This can be compared to a landscape with a vast number of hollows – in which you are looking for the deepest hole. A quantum computer should be able to find all the hollows more quickly and more efficiently than a conventional computer. In the real world, this solution might correspond, for example, to the optimum route for delivering parcels – the quickest and most efficient route uses the smallest amount of energy.

But the challenges facing the developers are not trivial: Quantum bits are by nature extremely sensitive to interference and must therefore be shielded almost perfectly from the outside world. The Rydberg atoms, for example, can be knocked out of step by the tiniest electric and magnetic fields. Vibrations too, caused by a passing lorry for example, can actually lead to a "quantum crash" of the computer. "We have to keep all these extraneous sources of interference under extremely close control," says Klaus Sengstock – hoping that, by the time project ends in November 2026, they will have a system on which first applications can be run in combination with conventional high-performance computers.

After that, it will probably take a few more years before the quantum annealer can be used for broader applications. Various parties have already expressed a concrete interest: A number of high-tech companies that develop lasers and optical systems are involved in Rymax, which is receiving a total of 29 million euros in funding. This also includes potential users, such as the Otto Group and the Hamburger Hafen und Logistik AG (HHLA). Cooperative ventures with DESY are planned as well: Quantum computing experts at DESY are already working on quantum algorithms that they hope to test on the Rymax computer one day.



Whereas a bit only takes on the values 0 or 1, a qubit can adopt any state between 0 and 1. Quantum physics allows for a superposition state: Much like an orchestra, in which the sound of each individual instrument is stored in the superposition of the sound waves, the superposition of the qubit can store any amount of information – clearly a great advantage over classical bits. Which superposition a qubit adopts depends on the physical problem that has been programmed. When the qubit is finally read out, it too always takes on a value of 0 or 1. The probability with which a value of 0 or 1 occurs is then the result of the quantum simulation of the physical system.

Picture: Claudia Höhne

Thanks to quantum technology, the 25 by 25 micrometre transition edge sensor (centre) could detect a laser pointer on Mars.

SENSITIVE **PROBES**

Quantum sensors open up a window to the unknown

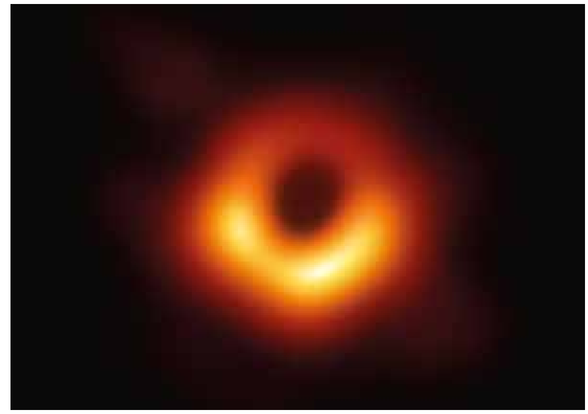
They are everywhere, yet barely visible: Sensors are playing an increasingly important role in technology. In cars they measure distances and acceleration, in smartphones they determine position and orientation, in industry they detect gases and hazardous substances. Thanks to quantum technology, sensors like these could soon become even more sensitive as they make use of some peculiar properties of the quantum world: Atoms behave like light waves and vice versa, and this makes new, sophisticated measuring techniques possible. And electrons – in atomic clocks, for example – can respond to the environment so sensitively as to register even the tiniest changes.

Expectations are therefore high: Quantum sensors are to serve as ultraprecise gravimeters in the search for mineral resources and in early-warning systems for earthquakes, and they could enable high-precision navigation devices, which are needed for autonomous driving systems, for example. Science is relying on the new technology too: Quantum sensors could help to detect hypothetical particles predicted by new theories, for example, and to examine the fundamental laws of nature – with higher precision than ever before.

"If you manage to harness quantum effects so as to use them in sensors, you can achieve a really amazing sensitivity," emphasises DESY physicist Steven Worm. Such quantum sensors are already providing valuable services in one particular area of science: radio astronomy in the millimetre and sub-millimetre range. This "astronomical window" allows scientists to observe, among other things, the formation of stars and the chemical composition of the gas clouds from which the celestial bodies are created. Here, it is superconducting receivers that make it possible to pick up the extremely weak radio signals. The spectacular first image of a black hole was also created using superconducting receivers. ››

Picture: PTB

Superconductivity is the phenomenon by which certain materials conduct electricity at extremely low temperatures without any losses at all. It is a typical quantum effect in which the very distinctive rules of quantum physics are apparent not only in the realm of atoms and molecules but also on a large scale, in our macroscopic world.



Peering into the gravitational chasm: The spectacular first image of a black hole would not have been possible without quantum technology.

Optical atomic clocks

But now other scientific fields are about to benefit from the new generation of sensors too – an experiment by the name of QSNET, for instance. "We are looking for super-lightweight dark matter candidates," Worm explains. "We want to use extremely sensitive quantum sensors to see whether fundamental constants of nature, which are generally considered to be immutable, do not after all vary a little over time." Such a variation could theoretically be brought about by the influence of certain extremely lightweight dark matter particles, in which case it would be a sign of their existence.

The quantum sensors that Worm and his team want to use are so-called optical atomic clocks, a recent refinement of conventional atomic clocks. These keep time with such great precision because they are based on an unchanging physical quantity: the radiation emitted by atoms when these are specifically excited, i.e. when energy is injected into them. This can be compared to tuning a musical instrument. A tuneable light source serves as a transmitter that shines light on the atoms, supplying energy to them. The atoms behave like a tuning device, matching the frequency of the transmitter to the value of their own radiation frequency. If it is too low,

The magnets of the ALPS II dark matter experiment have to be cooled down to minus 269 degrees Celsius using liquid helium while in operation.

Pictures: DESY, Heiner Müller-Elsner; Event Horizon Telescope Collaboration it is increased. If it is too high, it is reduced a little.

Conventional atomic clocks use microwaves. In optical clocks, on the other hand, which are a recent development, the transmitters are lasers. These shine light on the atoms with a frequency that is significantly higher than that of microwaves. This allows the clocks to keep time with one hundred times greater precision: Whereas the most accurate microwave clocks can be wrong by one second in 100 million years, it would take 10 billion years before the best optical clocks currently available were off by the same amount.

Miracle of precision

With the help of these miracles of precisions, the DESY team hopes to take a closer look at a particular fundamental constant, the so-called fine structure constant, commonly denoted by α (alpha). In physics, it quantifies the strength of the electromagnetic interaction. “We choose a clock that is particularly sensitive to alpha and compare it with a second clock that responds with a different sensitivity,” explains Worm. “By comparing clocks, we hope to determine whether alpha changes a little from time to time, due to a collection of dark matter particles passing through the clocks at that moment.” Several partners are involved in QSNET, including the Max Planck Institute for Nuclear Physics in Heidelberg.

In a tunnel at DESY, a special type of quantum sensor is also searching for ultralight particles – in the ALPS II experiment. The 250-metre-long setup is looking for a new, hypothetical class of particles: axions or axion-like particles. Certain theories in physics propose the existence of these extremely lightweight and ephemeral oddities. They too could be the answer to the mysterious dark matter that seems to populate the universe in vast quantities, but which until now

“We reckon that only a single particle of light will appear per day”

Friederike Januschek, DESY

has only revealed itself through its gravitational effects.

In order to detect these particles, which interact with almost no other matter, an international team led by DESY physicist Axel Lindner has come up with a clever experimental setup: “Theory predicts that the axions react very slightly with light,” he explains. “If we send a laser beam through a magnetic field, a tiny fraction of that light could be converted into axions.” Since these ghostly particles practically fail to interact with the rest of the world, they should be able to pass through any wall. Behind that wall, they could then change back into light – provided there is a strong magnetic field there too.

Light shining through a wall

The experiment designed by the ALPS team aims to exploit this “light shining through a wall” effect. It essentially consists of two evacuated magnetic sections, each a good 100 metres long and assembled using magnets taken from HERA, a decommissioned DESY accelerator. The magnetic sections are separated by a lightproof wall and enclosed by high-precision optical resonators. “We fire a laser beam into one half in the hope that some of the light will turn into axions,” explains Lindner. “The other half is in complete darkness. If a faint glow were to appear in it, this would have to come from an axion that had turned back into light.”

The challenges are enormous, though, because the light signals that the team needs to detect

Frederike Januschek working on the sensor used to search for dark matter made of axion-like particles

are extremely weak. “We reckon that only about one photon will appear per day – a single particle of light,” says Lindner’s colleague Friederike Januschek. “These are infrared photons, particles of light that carry a very small amount of energy.” In order to detect them, the experts have to prevent any light from entering the apparatus from the outside – that would lead to countless false alarms. At the same time, the sensors that are meant to register the telltale photon need to be extremely sensitive and reliable.

To this end, the group is relying on two separate methods: First, they are using a sensor that is closely related to the technology used in gravitational wave detectors, comparing a potential signal with a reference wave. In a second step, the scientists intend to install a special form of quantum sensor known as a transition edge sensor (TES). The underlying principle is that the sensor, which resembles a microchip, is cooled down to 100 millikelvins, ››

Picture: DESY

> *"If we send a laser beam through a magnetic field, a tiny fraction of that light could be converted into axions"*
> ***Axel Lindner, DESY***

a tenth of a degree above absolute zero at minus 273 degrees Celsius. At these extremely low temperatures, a quantum effect occurs in the sensor: superconductivity. Electric current then flows without any resistance.

Laser pointer from Mars

For ALPS II, the sensor developed at the US metrology laboratory NIST is set to operate at the boundary between superconductivity and normal conductivity. "In this range, its resistance depends strongly on the temperature," explains Januschek. "When the sensor captures a photon, it becomes a little bit warmer. This increases its resistance so much that we can measure the effect." The TES chip is so sensitive that it could, in theory, detect the light from a laser pointer shining on Earth from Mars. Another advantage is that, unlike most other light sensors, this one hardly ever sounds a false alarm in the dark – an important precondition for these measurements.

So far, the team has successfully tested its sensor chip. The tiny object is just 20 nanometres thick and has an area of 25 by 25 micrometres – making it much finer than a human hair. A special optical system will be used to collect the faint light signals and feed them into an optical fibre, which will then carry the signal to the chip. The quantum sensor is due to be installed in 2023. Until then, the apparatus will use the other type of sensor, based on the technology for gravitational wave detectors, to keep a lookout for the faint glow.

"We deliberately decided to use two different detection technologies," explains Axel Lindner. "Because if we detect a signal using both methods, we can be sure that it is indeed from an axion." This would be nothing less than a revolution for physics: The discovery would go far beyond the currently accepted theory of particle physics – the Standard Model – and could thus significantly expand our understanding of the makeup of our world.

GHOSTLY IMAGES FOR SCIENCE

"Ghost imaging" is to enable less destructive imaging

When you press the shutter release on a camera, a veritable torrent of light floods the camera chip with billions and billions of photons. In science, on the other hand, such a glut of light is not always desirable. Some objects – living cells, for example – do not take well to large amounts of light; they may be disrupted or even damaged by it. In order to take high-quality images without causing harm, DESY is working on a fledgling technique known as "ghost imaging", which makes use of the quantum properties of light.

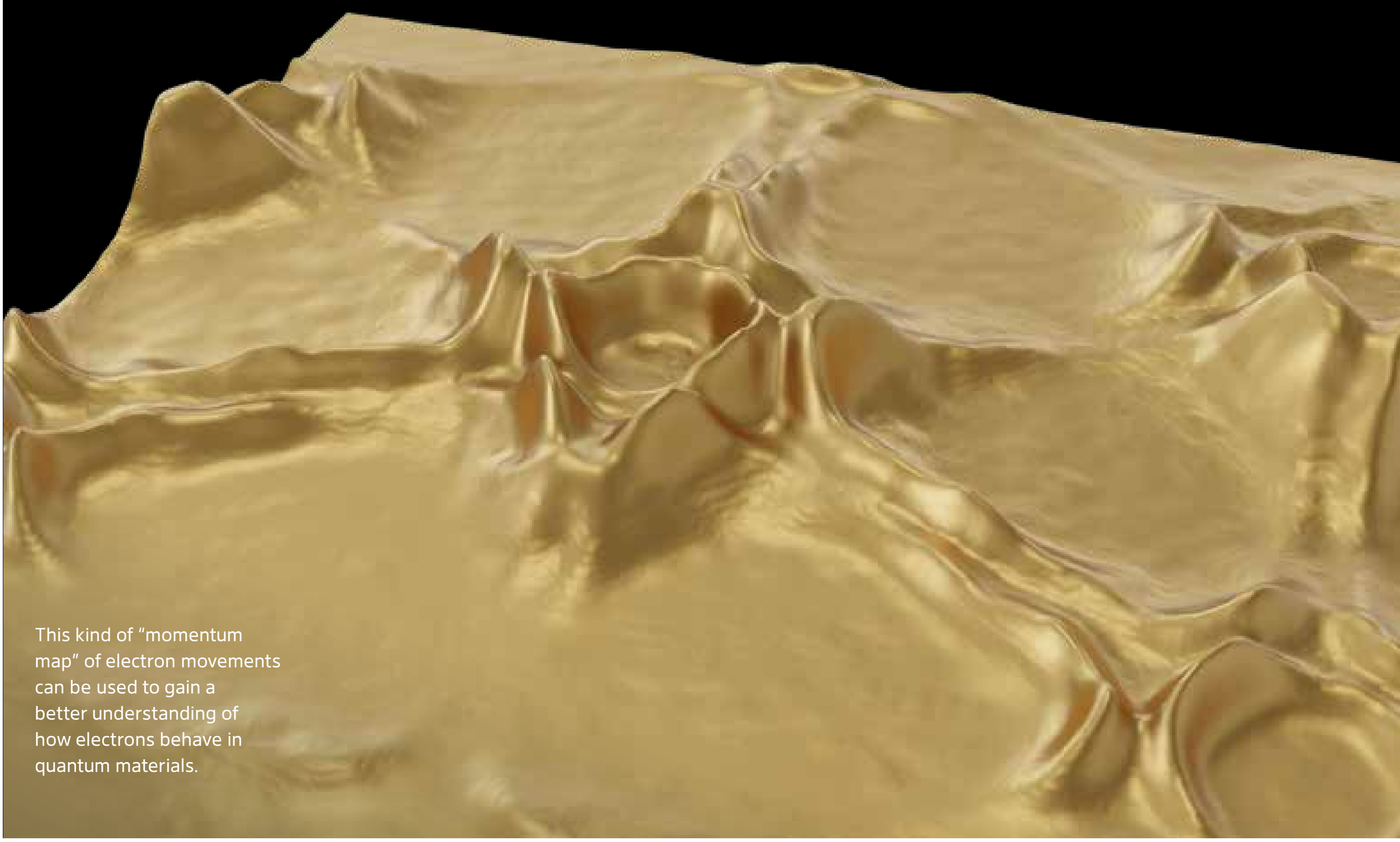
"The basic idea is to split an X-ray beam into two identical parts using a so-called beam splitter grating," explains DESY physicist Ivan Vartaniants. "The weaker part can be used to irradiate the sample without causing significant harm." In this case, it would be enough to use a detector that records the brightness of the light signal passing through the sample, but does not need to register its precise position. That measurement can be done by a different detector specialised in accurate spatial measurements. The really clever part is that this detector uses the signal from the other, more powerful light beam that has not actually "seen" the sample at all. Despite this, sophisticated computer algorithms can reconstruct the exact position where the weaker beam has passed through the sample. This is because, since both beams originated from the same place, i.e. the beam splitter grating, they are correlated with each other. Consequently, if the position of one beam is known, the position of the other can also be determined.

The scientists have already carried out some preliminary studies at DESY's X-ray laser FLASH. Over the coming years, they hope to determine how much of an advantage ghost imaging actually offers. "In the case of FLASH," says Vartaniants, "the goal is to look at the dynamics of living organisms at both high spatial and high temporal resolution."

Picture: DESY, Gesine Born

ASTONISHING PROPERTIES

Quantum materials make new applications possible



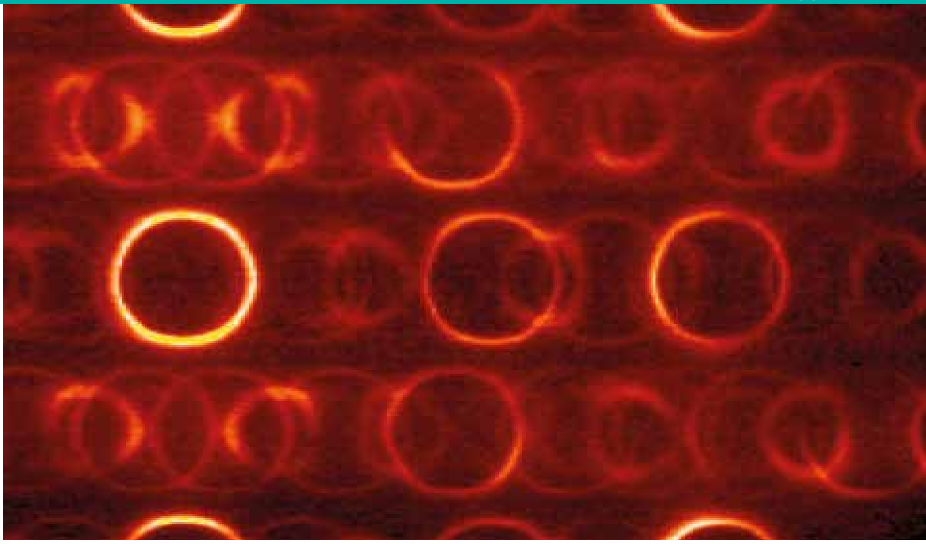
This kind of "momentum map" of electron movements can be used to gain a better understanding of how electrons behave in quantum materials.

Picture: DESY, AG Rossnagel

Computer chips that perform faster calculations and consume significantly less power. Cables that conduct electrical current loss-free at room temperature. And materials that allow high-performance quantum computers to be mass-produced. All these could be made possible by a fledgling class of materials known as quantum materials. DESY is using its X-ray sources to study the foundations and gather important basic knowledge for future practical applications.

From the outside, quantum materials do not look that different from any other material, but taking a closer look reveals that the electrons inside them interact unusually strongly with each other and also with the crystal lattice. That is why experts refer to them as "correlated materials". This close interaction leads to some strong quantum effects. These are not only expressed on the microscopic scale, but also very clearly at the macroscopic level. As a result, these materials display some highly unusual properties. "Often, it only takes a small change in temperature, pressure or electric voltage to dramatically alter the properties of the material," explains Martin Beye, interim scientific director of the free-electron laser FLASH at DESY. "For example, just adding a small amount of heat can turn something with a slightly bluish shimmer into a reddish shimmering lump of metal."

In some quantum materials, the spin of the electrons – their intrinsic angular momentum, so to speak – plays a key role: Simply put, the axis of rotation can either point up or down. This can be used to store and process bits, the basic units used by a computer: If "spin up" is a digital one, then "spin ›› down" is a digital zero. The really clever part is that, whereas in today's computer chips tiny currents flow through the conductors, the electrons could in future remain where they are and merely pass on their spin to their respective neighbours – like people during a removal who do not carry each box individually but instead form a chain and pass the boxes from hand to hand. With this approach, chips would conceivably require less energy because hardly any current would flow through them. This field of research is called spintronics, and some people already view it as a promising successor to today's electronics.



Colour-coded representation of the electron momentum – i.e. mass by velocity – in a misfit crystal, which has a high symmetry in only one direction.

Conducting bubbles

Martin Beye is working on yet another type of quantum material: alloys containing titanium oxide. "Using the X-ray sources at DESY, we were able to observe in detail how this material suddenly becomes electrically conductive under certain conditions," explains the researcher. "First of all, we observed small conductive bubbles in a large, non-conductive lake. But then the bubbles got bigger and bigger until they merged, and suddenly the entire sample became conductive." Such abrupt transitions could potentially be of interest for building novel electronic components, for example as the basis for a quantum computer.

While titanium oxide may not necessarily be suitable as a basic material for quantum chips, the fundamental insights emerging from the research provide clues as to how new electronic materials could be tailored. The planned ultimate X-ray microscope PETRA IV will allow even more detailed measurements to be made: "We could use it to observe the behaviour of the bubbles to an accuracy of just a few nanometres," says Beye enthusiastically. "Only when you can look that closely can you understand how a material like this really works."

Two-dimensional layered crystals of tantalum disulphide grown at Kiel University. This quantum material has a flaky structure similar to that of graphite.

Two-dimensional materials

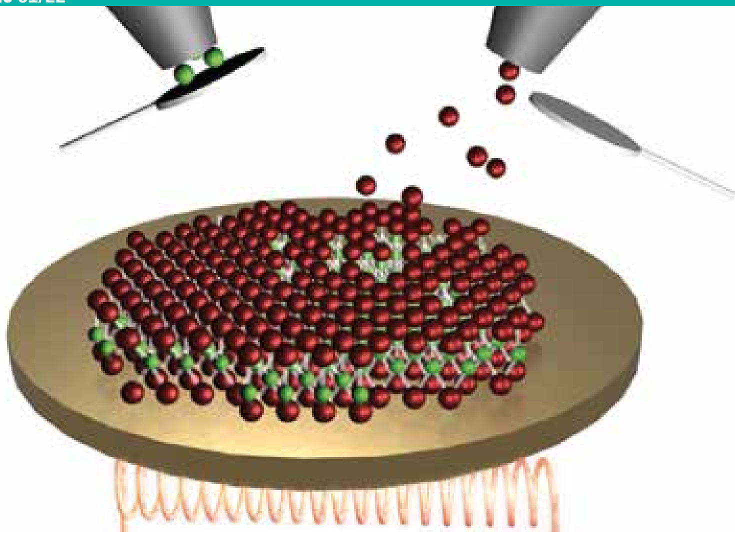
Another class of quantum materials is being researched by the DESY physicist Kai Rossnagel – materials that are extremely thin, being only a few atomic layers across. "Electrons can only move around them in two dimensions, which leads to some unusual quantum effects," he says. Graphene, for example – a two-dimensional form of carbon – is an exceptionally good conductor of electricity. Rossnagel, on the other hand, is interested in ultrathin sandwich structures: two so-called chalcogen layers on the outside, like slices of bread, while a special metal takes the place of the cheese in between them.

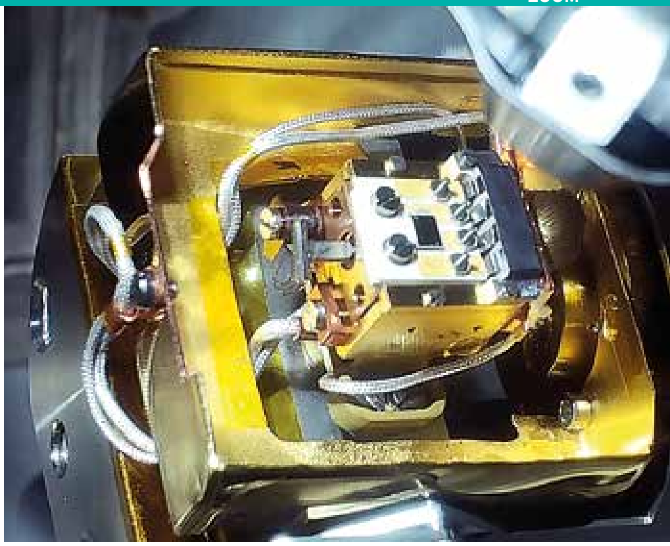
"Only when you can look that closely can you understand how a material like this really works"

Martin Beye, DESY

"Because these materials are so thin, they are easy to bend," explains the scientist. "So they could be used as smart patches, which you would stick on your skin and which would measure your body temperature or the oxygen

Picture: Kiel University, Julia Siekmann





Novel quantum materials can be tailor-made using molecular beam epitaxy by depositing individual atoms (here, for example, green: titanium atoms, red: selenium atoms) on a substrate under very clean conditions (in a vacuum), where they react to form a new material. Electronic components made of such materials can then be studied at DESY in detail during operation using photoelectron spectroscopy (right).

level in your blood." The processes taking place in such materials are in part extremely rapid – happening within femtoseconds, the millionth part of a billionth of a second. "If you want to observe them, you need very short pulses of light, like those provided by the two X-ray lasers FLASH and European XFEL in Hamburg," explains Rossnagel. "They make it possible to actually record stroboscopic films of the electrons' movements."

Nano-sandwiches

At the moment, the scientists are still exploring the physical foundations – but eventually such nano-sandwiches could become the basis of some spectacular applications. This is because, depending on the metal–chalcogen combination, they offer an enormous variety of electrical and optical properties. And since the layers can be stacked on top of each other in many different ways and twisted with respect to each other, this "sandwich Lego" permits an almost unlimited number of combinations. The perspectives this promises are fascinating: "Could this be used to design a superconductor that operates at room temperature and no longer requires any cooling?," Rossnagel wonders. It is true that materials already exist today that conduct electricity without any resistance. These are used in powerful electromagnets or special power cables. However, these components have to be elaborately cooled, using liquid nitrogen or helium, for example. If this cooling became unnecessary, superconductivity would be significantly cheaper and interesting for other applications.

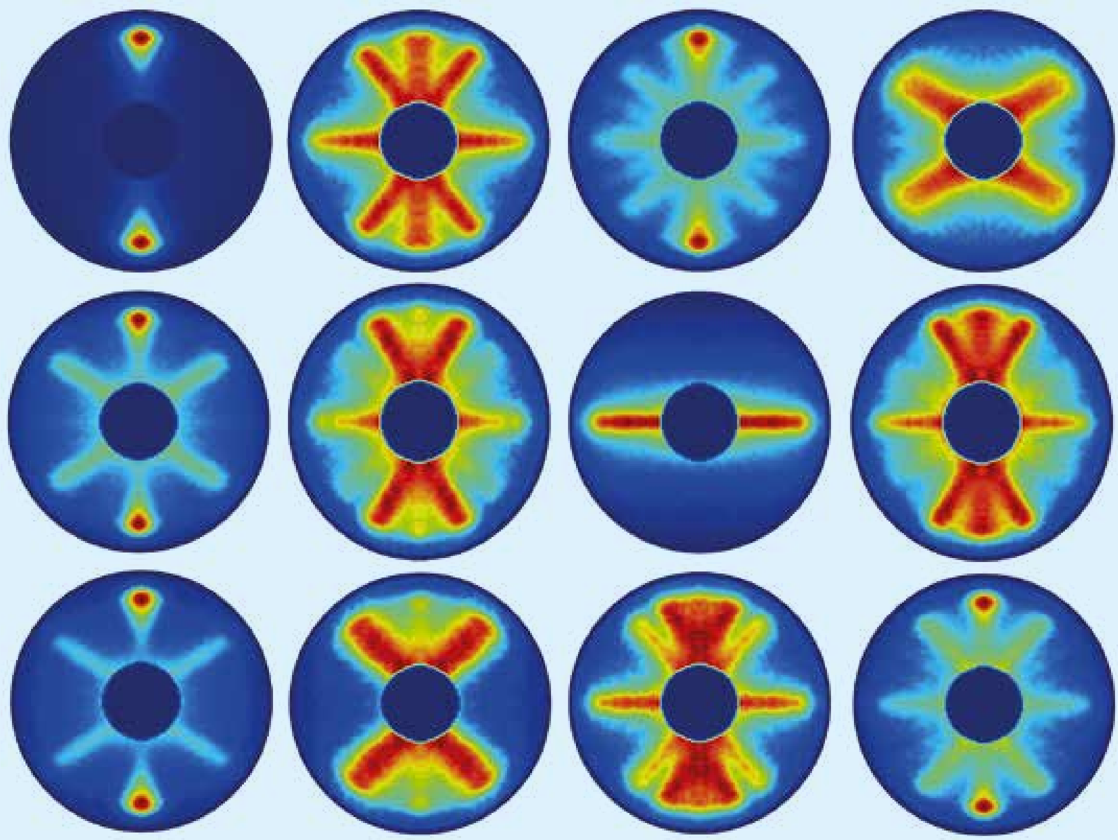
"They make it possible to actually record stroboscopic films of the electrons' movements"

Kai Rossnagel, DESY

Qubits in a tiny space

Another vision is that these two-dimensional materials could one day serve as qubits, the fundamental elements of a quantum computer. The hope is that this would make it possible to fit millions of qubits into a very small space – ideally, a quantum chip could be made to fit inside a smartphone. However, before that happens, various fundamental questions need to be sorted out: What exactly are these qubits supposed to look like? How can they be made so robust that they do not lose their quantum information prematurely? And how can such vast numbers of qubits be reliably accessed and read out? "DESY's X-ray sources are excellent and unique tools for analysing the properties of such systems with great precision," says Kai Rossnagel. "This will allow us to make many more contributions to quantum materials research in the future, no doubt for industry too."

Pictures: DESY, AG Rossnagel; DESY, Marta Mayer (portrait)



Quantum-mechanical rotation of a carbonyl sulphide molecule, recorded at intervals of about seven picoseconds. The colours indicate the probability of the rod-shaped molecule being in a particular position.

THE QUANTUM **TAMERS**

Sophisticated tricks allow quanta and quantum systems to be carefully controlled

Quantum systems are usually highly sensitive and therefore predestined to be used as powerful sensors and in revolutionary computer architectures, for example. But their high sensitivity is also their weakness: Even the slightest disturbance can throw quantum systems off balance. This is why it is important to have them as under the best possible control: quantum control. Researchers have come up with a variety of tricks to successfully tame quanta. This has opened up new perspectives for measuring time extremely precisely and for recording high-precision "films" of molecular reactions.

A group led by DESY researcher Ralf Röhlsberger, for example, has been using a sophisticated method to control the internal oscillations of iron nuclei and their emitted radiation with enormous precision – to within 1.3 zeptoseconds, or one thousandth of a billionth of a billionth of a second. To do this, the team excites the nuclei of the iron atoms in an ultrathin magnetic material using pulses from the X-ray source PETRA III. At the same time, they send in a microwave – resulting in a short magnetic pulse

> *"With this, we have given science a new analytical tool"*
>
> ***Jochen Küpper, DESY***

travelling through the material. This in turn affects the behaviour of the iron nuclei in such a way that the internal oscillation is shifted by 1.3 zeptoseconds compared with the situation without the additional magnetic pulse. The team then uses sophisticated detection techniques to precisely measure this tiny time lag.

Ticking of the nuclear clock

Magnetic pulses can thus be used to specifically control quantum systems – in this case, oscillating iron nuclei. It seems feasible that, in the future, this could be used to accurately set a new generation of ultraprecise clocks, so-called nuclear clocks. These are based on the oscillations of atomic nuclei and should "tick" away with much higher precision than today's atomic clocks. In principle, the knowledge

Picture: DESY, Evangelos Karamatskos

gained at DESY could help scientists to readjust and hence stabilise these clocks, for example, in the event of minute temperature fluctuations. The same is conceivable for certain types of qubits, so-called diamond defects. Here, too, the qubits – the fundamental processing units of quantum computers – could be precisely readjusted.

The team led by DESY physicist Jochen Küpper has mastered a different kind of quantum control: It has managed to make molecules freely suspended in a vacuum chamber rotate or to spatially align them with great precision – such quantum choreography is an important prerequisite for being able to film the extremely rapid behaviour of these molecules. Although it has been possible for some time now to hold and align even complex molecules with laser pulses as if with tweezers, this requires the laser to be active all the time, which is highly disruptive when conducting certain types of experiments, especially studies of chemical dynamics. "We have developed a new technique where, after aligning the molecule using a laser pulse with a long rise time, the laser is quickly switched off again," explains Küpper. "This allows the aligned molecule to be studied without disturbances by the laser field."

Fit for the Guinness Book

The team succeeded in getting carbonyl sulphide – a rod-shaped molecule made up of oxygen, carbon and sulphur – to rotate by giving it a brief laser kick. Afterwards, they were able to literally film the quantum-mechanical rotation of the molecule using a special detection method. The result is an extremely short film, consisting of 651 individual images recorded in 120 trillionths of a second, which even made it into the Guinness Book of Records and corresponds

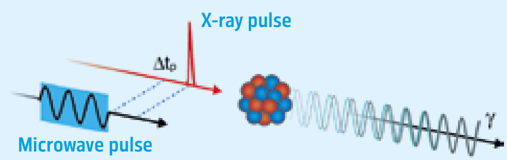
Ralf Röhlsberger is studying magnetism and so-called coherent phenomena.

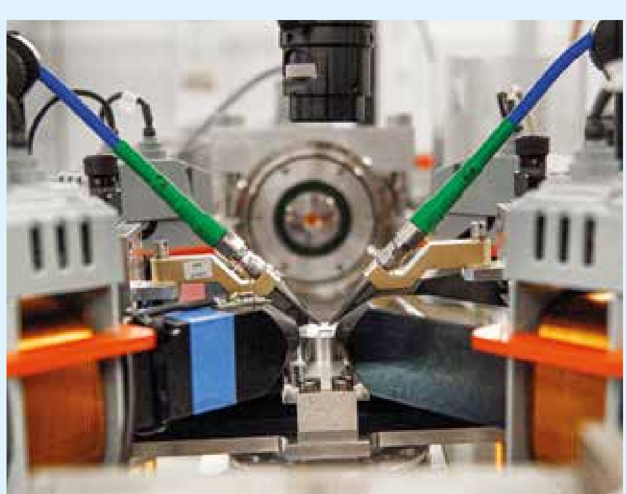
to recording an entire "quantum carpet". In addition, in an electron diffraction experiment based on these results, the team was able to determine the length of the chemical bonds in carbonyl sulphide to within five trillionths of a metre – another world record.

Recently, the group has managed to further refine its technique and align a more complex structure by laser pulse: the biomolecule indole. This plays a role in the absorption of ultraviolet radiation in the skin, among other things, for example in developing sunburn. "One challenge was to switch off our lasers quickly enough once they had aligned the indole," explains Küpper. Only a small window of time is available after switching them off before the molecule twists out of alignment again. But the time is long enough to excite the indole using ultraviolet radiation and to measure its response by ingenious methods. In order to resolve the individual components of the molecule, it is necessary for the alignment to be as precise as possible – it makes a substantial difference to the analyses whether the molecule is "standing up" or "lying down".

The experts were recently able to show that they had successfully aligned the indole. Now they are working towards their actual goal: to identify the individual atoms in the aligned molecule and what role each of them plays in the reactions. "In principle, this technique could be used to align and study all kinds of molecules, such as vitamins or neurotransmitters," Küpper believes. "This means that we have given science a new analytical tool with which to understand the properties of such molecules in more detail in the future."

Schematic diagram of the experimental setup: An atomic nucleus is excited by means of an X-ray pulse and emits gamma radiation. If a second excitation with a microwave pulse (front left) produces a so-called magnon oscillation in the solid, the oscillation of the atomic nucleus – and hence of the gamma radiation – experiences a time delay on the order of zeptoseconds.





Zepto clock generator: The sample on the circular platform in the centre of the picture is connected to microwave measuring tips. The X-rays it emits are analysed at the end by a detector. Electromagnets with iron yokes around the sample platform create a magnetic field at the sample location in order to align the magnetisation inside the sample.

Picture: DESY, Lars Berg

femtopolis

QUANTUM TECHNOLOGY CATCHES UP WITH SCIENCE FICTION

In Anton Zeilinger's laboratory, science fiction dreams are coming true: The Viennese quantum physicist and his team have turned teleportation into a reality. For the moment, though, it only works on subatomic particles. To achieve this, the Austrian researchers used entanglement, an effect that Albert Einstein referred to dismissively as spooky action at a distance. According to the rules of quantum physics, two particles can be entangled to form a common state that can only be described as a whole, but not by the sum of the two components.

What makes the phenomenon so special is that the two particles can be separated in space without destroying the entanglement. When one of the two particles is manipulated, the other will change as a result, even over long distances. This is how Zeilinger's team "beamed" the quantum state of a photon (a particle of light) under the Danube already 20 years ago. Unlike in the starship "Enterprise", quantum states are transmitted rather than the particles themselves. However, the outcome is the same: An exact copy is created, while the original is destroyed.

In the meantime, teams all over the world have also performed such quantum teleportation and shown that it not only works for massless photons, but also for particles having a mass, such as electrons. For the time being, however, transporting human beings by beaming them remains science fiction. The information about a person's quantum states that would have to be transmitted would fill a stack of CDs 1000 light years high, as Zeilinger once calculated. Even using the fastest data transmission conceivable today, it would be quicker to walk.

Despite this, quantum teleportation is not futile. It can be used to achieve communication that is secure against eavesdropping for physical reasons. This is because, since quantum states cannot be cloned, i.e. the original is always destroyed when a copy is made, any eavesdroppers on the line would immediately give themselves away. Moreover, quantum teleportation could provide a way for quantum computers to communicate with each other.

Teleportation by beaming is not the only science fiction feature that can be implemented with the help of quantum physics. For example, a research team has used DESY's X-ray source FLASH to produce aluminium that is transparent, like that created by the Enterprise's chief engineer Scotty in "Star Trek IV – The Voyage Home". Unlike in the cinematic adventure, however, the aluminium in the FLASH beam remained transparent only for fractions of a second and also only to X-rays of a certain wavelength. The transparency was brought about by saturating the aluminium's absorption using an extremely intense X-ray beam – the metal atoms were simply unable to absorb any further radiation, allowing it to pass through unimpeded.

In another experiment, a group led by DESY researcher Ralf Röhlsberger succeeded in making iron transparent as well. Here, the entanglement of the atoms in two thin layers of iron played the central role. The layers were placed between two tiny X-ray mirrors, between which a standing X-ray wave was formed. One layer of iron was placed on the crest of the wave, the other in the trough. If the atoms in the two layers are entangled, then the iron becomes transparent. Again, the effect only lasted for a fraction of a second, but according to Röhlsberger it could prove useful for developing quantum computers, including optical switches.

Picture: Forschungszentrum Jülich GmbH

Tommaso Calarco is the head of the Peter Grünberg Institute for Quantum Control at Forschungszentrum Jülich. He is one of the initiators of the billion-dollar Quantum Flagship programme with which the EU is promoting quantum technologies in Europe.

femto: The European Union's Quantum Flagship programme was launched in October 2018. What was the motivation behind it, why was this initiative set up?

Tommaso Calarco: There was, at the time, already a great deal of scientific expertise in quantum technologies in Europe, but there was an investment gap: Unlike big companies especially in the USA, European industry did not really want to invest in this future technology yet. So the public sector had to step in to stimulate such investments. The Quantum Flagship programme was designed to run for ten years; altogether, it was supposed to have a volume of half a billion euros, half from the European Commission and the other half from the member states.

femto: The Quantum Flagship programme has been running for a good three years now. What has been happening during this time?

"WE EXPECT TO SEE A **REALLY POWERFUL** QUANTUM COMPUTER WITHIN 10 TO 15 YEARS"

Tommaso Calarco: A lot has happened. We are seeing the first benefits, both scientific and industrial. Some of the world leaders in quantum computing and quantum communication are now established in Europe. Industry initiatives have been set up, such as the European Quantum Industry Consortium, or QuIC for short. And several start-ups have been created that sell quantum computers, in Austria, France, Finland and Germany, for example. In addition, the Quantum Flagship programme has been expanded considerably. The EU is going to invest an additional almost two billion euros by 2027, on top of further programmes by its member states, for example by France, Italy and Germany. In total, we will not be investing one billion euros in quantum technologies over the next few years, but seven billion!

femto: Has this made up for the head start that the USA and perhaps China had?

Tommaso Calarco: There are still areas in which the USA is ahead of us, especially when it comes to quantum computers using superconducting qubits. Google and IBM have gone to a lot of effort there, and we have been able to gain on them, though not quite catch up yet, but we are well on our way. In other areas, such as quantum simulators based on neutral atoms, we have now drawn level, however.

femto: What will be important in the coming years when it comes to turning the research results into practical applications?

Tommaso Calarco: In quantum computers, we need to increase the number and the quality of the qubits. A higher number alone is not enough: We need high-quality qubits with low error rates. It is true that Google and the Chinese Academy of Sciences have been able to demonstrate that a quantum computer can solve specific problems much faster than a supercomputer. But, for the time being, these problems are of a more academic interest. We now want to show that a quantum computer can also tackle problems that are of commercial interest. At the same time, there are challenges on the software side, especially in terms of dovetailing with high-performance computing and offering cloud services to industry.

femto: When could quantum technologies really take off?

Tommaso Calarco: In quantum communication, we expect this to happen in three to five years: The outline of a communication infrastructure will be in place and the first sections of it will exist. We expect to see a really powerful quantum computer within 10 to 15 years. However, special-purpose applications, such as quantum simulations of materials or chemicals, might be of practical use already in five to seven years.

femto: Countless activities are taking place in the realm of quantum technology in Europe right now, both at universities and in industry. Are they all being coordinated well enough, or is there room for improvement?

Tommaso Calarco: At the EU level, the scientific community is well connected, thanks also to the Quantum Flagship programme. Something we want to promote even further is dovetailing with industry. But so many industry players are currently showing an interest in quantum technologies that we are optimistic that this will continue to develop favourably.

EU Quantum Flagship programme: https://qt.eu

Disruptive potential

Quantum technologies offer fantastic prospects for the economy and for society

Quantum technologies hold promising opportunities for science, industry and society. They are expected to solve complex problems more quickly and above all better, to work out new drugs and to reposition measurement technology and imaging processes for applications ranging from medicine to environmental technologies. Those are just a few of the many conceivable applications that many researchers around the world are already working on today. It has been estimated that quantum computing, for example, will transform entire industries by 2040 and generate an estimated turnover of up to 850 billion dollars (about 767 billion euros). The technology is expected to have extreme economic clout.

And not just in the distant future either. Though experts believe that it will take at least 10 to 20 years before the most prominent example of quantum technology – the quantum computer – becomes widely used, the first prototypes already indicate that computing with the help of so-called qubits is in fact much faster and can accomplish more complex tasks than using classical bits. It is now a matter of eliminating their susceptibility to errors and increasing their computational capacity.

"If you want to establish a new technology, you need staying power"

Arik Willner, DESY

Funding and implementation problems

Concrete applications of quantum technologies are already closer in areas such as communications, sensor technology and materials science: Modern lasers and transistors are already making use of them today. "Quantum technologies have already arrived in our reality," says Michael Bolle, former member of the German government's Council of Experts on Quantum Technology and former Managing Director, Chief Technology Officer and Chief Digital Officer of Robert Bosch GmbH. "However, because such technologies have much more potential for the future and can be disruptive, it is important – for both government and industry – to invest massively in them now."

Pictures: iStock; DESY, Axel Heimken (portrait)

In its "Roadmap Quantum Computing", the Council of Experts recommends that it is an absolute "must do" for a leading technology site to help drive such developments forward. "Germany is in a very good position here in terms of fundamental research," adds Bolle. "But when it comes to transferring knowledge to concrete industrial products, for example entire quantum computers, the USA and Asian countries are way ahead of us." While funds are now amply available, "we have an implementation problem: How do we orchestrate the many different players in research and industry – also across Europe – so as to use the funds efficiently?" The roadmap makes suggestions on this, recommending that new hubs and competence networks should be set up, as well as the umbrella organisation "German Quantum Community".

"Quantum technologies have already arrived in our reality"

Michael Bolle, Chairman of the Board of Trustees of the Carl Zeiss Foundation and former member of the German government's Council of Experts on Quantum Technology

Bridge to industry and society

DESY, of whose Innovation Advisory Committee Michael Bolle is a member, would like to lead the way: "It can serve as a bridge between fundamental research, industry and society," says Bolle. The research centre has highly skilled scientists in this field and a lot of experience with transferring knowledge to industry. "We have the experts; we have the large-scale facilities for studying quantum materials; and with Science City Hamburg Bahrenfeld, we already have, in effect, an ecosystem in which we can collaborate with partners such as the Max Planck Society, the Hamburg University of Technology and the Hamburg University of Applied Sciences, as well as with various companies, and in which start-ups can get off the ground," says DESY's Chief Technology Officer (CTO) Arik Willner.

In addition, with the unique technical capabilities of its large-scale research facilities, DESY could contribute to the standardisation and quality assurance of quantum technology. "Our X-ray facilities can be used, for example, to precisely measure whether a quantum device responds and operates exactly as it is meant to," explains DESY's CTO. In addition, physicists, engineers and computer scientists – the next generation of quantum technicians – can be trained at DESY. The DESY manager also believes that a separate course of study in quantum technologies is possible in Hamburg.

From "push" to "pull"

DESY is already engaged in a close dialogue with universities, academic and industry players, such as the new DLR Innovation Centre for Quantum Technologies in Hamburg. DESY itself is focusing its various activities in the DESY Quantum initiative. "The seeds have been sown," says Willner. What is needed now is perseverance. For public-service investors, this also means: Don't let the success stories you hear in the meantime from the USA or China make you nervous. "If you want to establish a new technology, you need staying power – and long-term funding that doesn't dry up halfway through."

According to the Council of Experts, writing in its roadmap, this is how the transition from "push to market", i.e. the dependency of a new technology on subsidies, to "market pull" can be successful: The technology site becomes so attractive that it draws in companies and funds. "The world will not wait for Germany," warns the Council of Experts. "We have to start now."

Picture: Private

REVOLUTIONARY CONSEQUENCES

The term "disruptive" is used to describe the impact of a new technology that revolutionises a specific sector or even society as a whole. It is meant to emphasise that the technology in question brings something radically new to the game, and it is often used synonymously with "revolutionary". While the term is a popular buzzword today, experts do indeed expect some genuine disruptions from quantum technology – because it will not only revolutionise computing, but probably also many other technical disciplines as well as areas of society. We can expect a far more detailed understanding of different areas of nature, of life at a molecular level and of the brain. Experts believe that medicine will benefit just as much as logistics and mobility. **"However, the truth also includes the fact that quantum technologies could be misused,"** says Michael Bolle, "to hack complex encryption, for example." Aside from opportunities, the brave new quantum world thus also harbours potentially disruptive threats.

SPECTRUM

News from research

Two-photon technique: After the absorption of an X-ray photon, the water molecule can bend up so far that after only about ten femtoseconds (quadrillionths of a second) both hydrogen atoms (grey) are facing each other, with the oxygen atom (red) in the middle. This motion can be studied through the absorption of a second X-ray photon.

X-ray laser reveals how radiation damage arises

An international research team has used the European XFEL X-ray laser to gain new insights into how radiation damage occurs in biological tissue. The study reveals in detail for the first time how water molecules are broken apart by high-energy radiation, creating potentially hazardous radicals and electrically charged ions, which can go on to trigger harmful reactions in the organism. Since water is present in every known living organism, the splitting of the water molecule H_2O by radiation, called the photolysis of water, is often the starting point for radiation damage.

The team led by Maria Novella Piancastelli and Renaud Guillemin from the Sorbonne in Paris, Ludger Inhester from DESY and Till Jahnke from European XFEL shot the X-ray laser flashes at water vapour and analysed the reaction using a new technique. As the results show, the disintegration of the water molecule is much more complicated than initially expected. The molecule starts to stretch and expand before eventually breaking apart. After only ten femtoseconds (quadrillionths of a second), the two hydrogen atoms (H), which are normally attached to the oxygen atom (O) at an angle of 104 degrees, can build up so much momentum as to face each other at an angle of around 180 degrees.

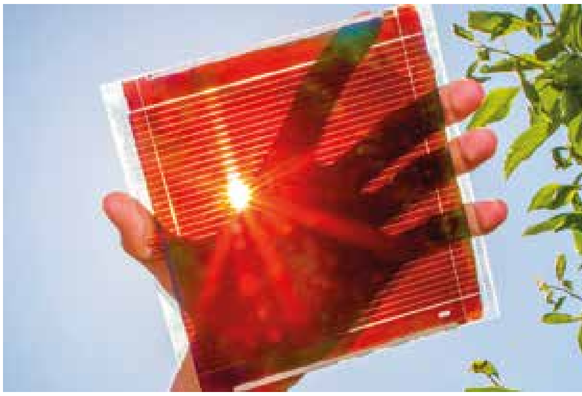
As a result, the oxygen atom is not in fact flung away hard when the molecule breaks up, because the momenta of the two hydrogen nuclei largely balance each other out as they fly off, leaving the oxygen virtually at rest in the middle. In an aqueous environment, this free oxygen radical can then easily lead to further potentially harmful chemical reactions.

“The disintegration of the water molecule is an important first step in the further chain of reactions that ultimately lead to radiation damage,” explains Inhester, who works at the Center for Free-Electron Laser Science (CFEL), a collaboration between DESY, Universität Hamburg and the Max Planck Society. The newly gained insights address elementary questions about reaction dynamics in water, which are to be further investigated at the Centre for Molecular Water Science (CMWS) currently being set up with international partners at DESY.

Physical Review X,
DOI: 10.1103/PhysRevX.11.041044

Pucture: DESY, Ludger Inhester

Atmosphere changes stability of novel solar cells



Solar cells made of perovskite are a promising alternative to the conventional variants made of silicon.

An international team of scientists led by the Technical University of Munich (TUM) has used DESY's X-ray source PETRA III to observe for the first time how different atmospheres affect the operation of novel high-performance solar cells made of perovskite. The researchers discovered that vacuum leads to the rapid degradation of the structural composition and thus also of the efficiency of the cells, whereas a nitrogen atmosphere stops this degradation.

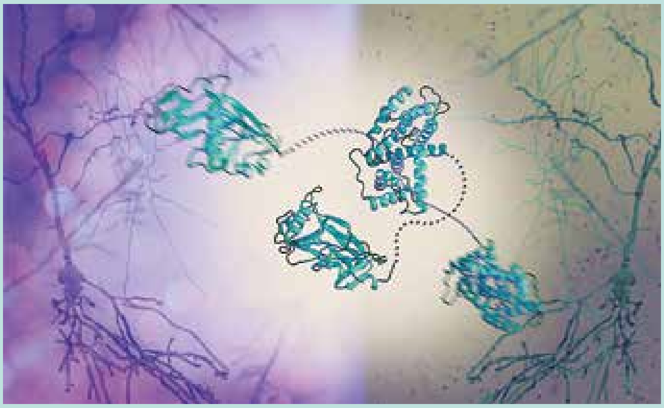
Perovskites are very common minerals. In the past ten years, researchers have been able to increase the efficiency of perovskite solar cells from 3.8 percent to 25.5 percent, making them competitive with single-crystal silicon solar cells. However, the main obstacle to industrialisation is the low long-term stability of the cells. Within a few hours, the electricity yield can drop dramatically because the nanostructure of the crystals changes and they segregate.

The research group, led by TUM researcher Peter Müller-Buschbaum, has now shown that different inert atmospheres can accelerate or suppress degradation pathways for perovskite solar cells. The discovery could improve test protocols for experiments on the long-term stability of perovskite solar cells and raise awareness of such effects in other studies as well, the team writes.

Nature Energy,
DOI: 10.1038/s41560-021-00912-8

Picture: TNO

Herpes viruses have “handcuffs”



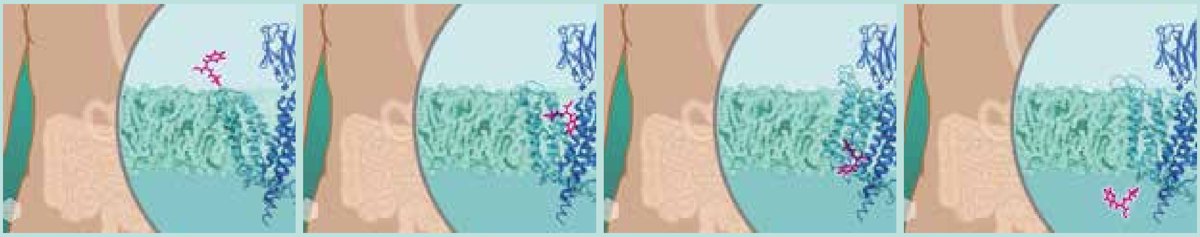
Many viruses have specialised proteins to reprogramme host cells. Thanks to its great flexibility, the viral protein pUL21 can control not just one but many host proteins.

Picture: EMBL, Isabel Romero Calvo

Herpes viruses put a kind of molecular handcuffs on certain proteins in infected human cells to force them to perform desired actions. This is shown by studies conducted by the European Molecular Biology Laboratory (EMBL) at DESY's X-ray light source PETRA III. The researchers, led by EMBL group leader Dmitri Svergun as well as Stephen Graham and Colin Crump from the University of Cambridge, investigated the effect of herpes simplex virus 1 (HSV-1) on so-called phosphatases. These belong to the production managers in the cell that switch other proteins on and off as needed.

The experiment shows that a viral protein called pUL21 binds phosphatase and other human proteins that are involved in protein secretion. According to the study, pUL21 is shaped like a flexible string with rigid components at each end, which bind other proteins. It chains the human phosphatase 1 bound at one end to another protein at the other end, just like handcuffs. By bringing the two proteins close together, pUL21 forces the phosphatase to steer the activity of the other protein, which in turn supports the production and release of viral copies from the cell.

“Understanding how the viral protein behaves and interacts with human proteins may help design new drugs and vaccines against herpes,” Graham says.



PepT1 is a versatile peptide transporter that can move many molecules through the gut wall into the blood.

Structure of transport protein should enable better drugs

A team from the Centre for Structural Systems Biology (CSSB) at DESY has decoded the structure of an important nutrient transporter in the human intestine. The protein PepT1 is located in the gut wall and transports small molecules from food into the bloodstream so that our body can use these so-called peptides to build its own new proteins.

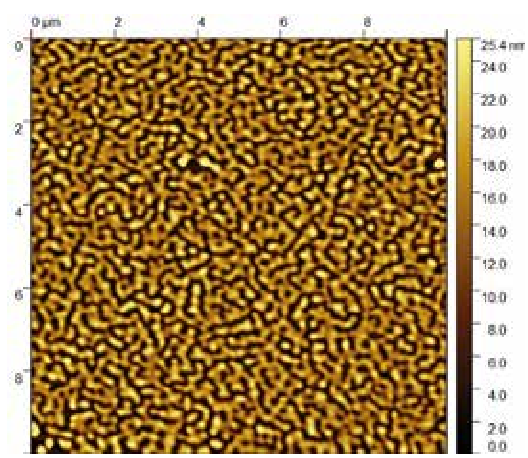
PepT1 not only transports food peptides, but also various types of drugs, for example antibiotics, antivirals and drugs against high blood pressure. However, PepT1 transports the drugs less efficiently than it does many of the natural peptides. As a result, only a fraction of the drugs we ingest enter our bloodstream. The rest remains in the gut, which can lead to various side effects.

"Currently, it's almost impossible to predict whether a drug candidate can cross the gut wall via this transport system," says Christian Löw from the European Molecular Biology Laboratory (EMBL), who led the study together with Thomas Marlovits from DESY and the University Medical Center Hamburg-Eppendorf (UKE). "Now that we know what the PepT1 structure looks like, it will be possible to design new drugs that exploit PepT1 to cross the gut wall much more efficiently than before."

Science Advances,
DOI: 10.1126/sciadv.abk3259

Picture: EMBL, Isabel Romero Calvo

Flexible and transparent magnets



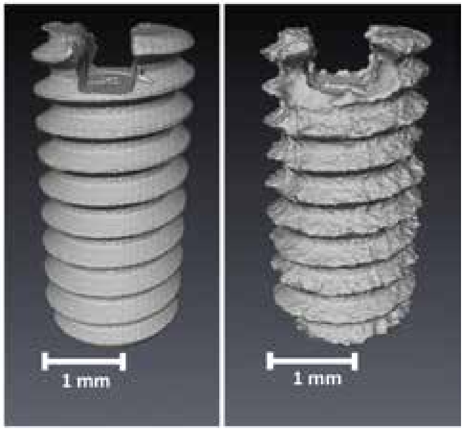
Atomic force microscope image of a magnetic thin film of organic radicals

A new class of organic magnetic materials promises innovative applications and could provide a sustainable alternative to metal magnets containing rare earths. At DESY's X-ray light source PETRA III, an international team has demonstrated magnetism in purely organic thin films for the first time. The researchers studied so-called organic radicals – carbon compounds that carry an unpaired electron. This results in a permanent magnetic moment that is not due to the effect of an external magnetic field.

"In the past, magnetism in purely organic radicals was known only for crystals and it was completely unknown in thin films," explains Maria Benedetta Casu from the University of Tübingen, who led the research. However, thin films are usually necessary for applications. Using a clever combination of low temperatures and a strong magnetic field, the team has now been able to show that the radical thin films do indeed exhibit long-range magnetism and that their magnetic behaviour can even be influenced by the conditions during production. "These results open the way to the advent of flexible, light and transparent magnets and thus to a variety of new futuristic applications," Casu emphasises.

Chem, DOI: 10.1016/j.chempr.2021.11.021

Picture: University of Tübingen, Maria Benedetta Casu



The investigation at DESY's X-ray light source PETRA III showed after 56 days (right) that the tips or teeth of the screw thread are the first to dissolve and gradually become rounded. In contrast, corrosion does not progress as strongly in the thread valleys.

Wanted: corrosion

Bone screws and plates that dissolve on their own after a broken bone has healed promise great benefits – they could save many a patient from having to undergo follow-up surgery. A research team led by Helmholtz-Zentrum Hereon has now used a 3D X-ray method to quantitatively determine for the first time how different magnesium alloys dissolve over time under body-like conditions.

The researchers produced screws from two different alloys, one with five percent gadolinium, the other with ten percent. They placed these samples in Petri dishes filled with body fluid-like mixtures of salts, vitamins and proteins and exposed them to body-like conditions in incubators for 56 days. During this time, they examined them several times at DESY's X-ray light source PETRA III.

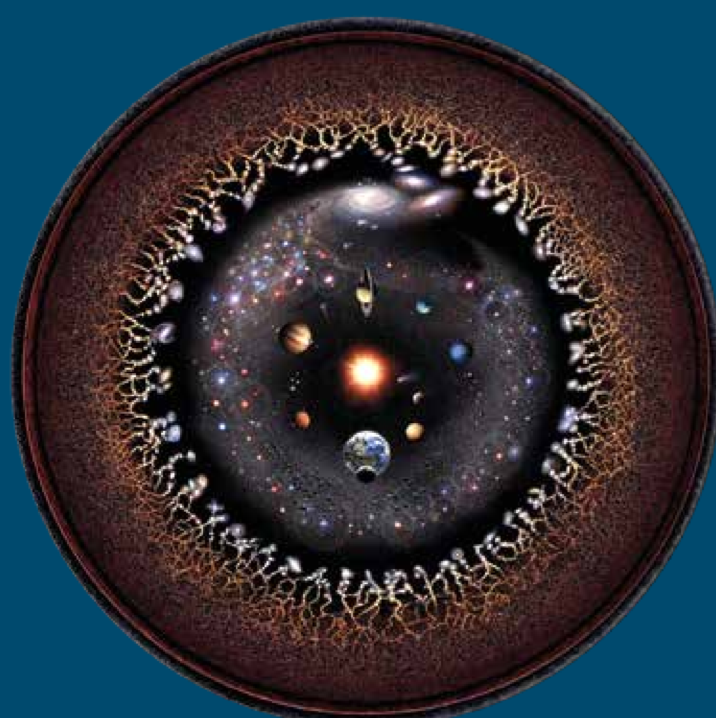
"The magnesium alloy with five percent gadolinium corroded much faster than the one with ten percent," says Wiese. Extrapolating, a screw with low gadolinium content would have completely dissolved in the body after just over four years. A screw with more gadolinium, on the other hand, would only have disappeared completely after about eight years. This means that, if long-term stabilisation is required after a bone fracture, it is better to implant magnesium screws with higher gadolinium content.

Journal of Magnesium and Alloys, DOI: 10.1016/j.jma.2021.07.029

femtomenal

46 600 000 000 LIGHT YEARS HORIZON.

Standing on a high dune by the sea, you have a horizon of perhaps 20 kilometres. In space, the horizon extends considerably further: Our current knowledge suggests that the boundary of the observable universe is located at a distance of around 46.6 billion light years. This is significantly further than light has been able to travel during the existence of the cosmos, currently aged 13.8 billion years. However, space itself has continued to expand since the Big Bang, like dough left to rise, and so the boundary of the observable universe has moved further and further away. In the process, the expansion of space has also stretched the light waves themselves, so that distant objects appear to have longer wavelengths, making them redder than they actually are. Astronomers call this effect the cosmic red shift, and it can be used to determine how far away an object is.



In this artist's impression, the South American Pablo Carlos Budassi has depicted the observable universe on a logarithmic scale – from our solar system in the centre past the neighbouring star Alpha Centauri, the Milky Way, its neighbouring galaxy Andromeda and more distant galaxies to the so-called cosmic web, the cosmic background radiation and the plasma state shortly after the Big Bang.

Radiolaria
model

An unusual alliance between physicists and marine biologists is putting heavy magnets on new feet

Artistic: Close-up of the irregularly shaped prototype of a magnet support frame for PETRA IV

Picture: DESY, Christian Schmid

Radiolarians are among the smallest creatures in the world. The largest of them can only just be seen with the naked eye, as tiny dots. These protozoa are not capable of independent locomotion but instead drift with the current near the surface of the sea and feed on particles caught in their "spikes" – elongated outgrowths of their endoskeleton pointing in all directions. Anyone looking at Ernst Haeckel's drawings, which the famous naturalist made in the 19th century from photographs taken through a microscope, will be fascinated by the variety of filigree shapes displayed by these tiny creatures. Their radial protrusions are supported by thin spines made of silicon dioxide and finely branched microtubules made of proteins. Some specimens look like ice crystals with their symmetrical arms, others resemble ornamental brooches or roundish bees' nests with hexagonal honeycombs in their centre and spikes on the outside.

It is hard to believe then that these tiny, delicate creatures, which have populated our oceans since time immemorial, are to serve as a model for the construction of a kilometre-sized particle accelerator facility with its massive high-tech machines. But that is indeed the case: Some vital components of the new high-resolution 3D X-ray microscope PETRA IV, which is to be built at DESY in Hamburg over the coming years, will probably mimic the structure of radiolarians.

The components in question are the frames that will support the magnets that keep the particle beam travelling along its circular path. These steel tables, known in the field as girders, are about three metres long and 60 centimetres wide; they weigh tonnes and so provide an unshakeable, solid foundation. "But conventional support frames are no longer able to provide the extreme precision required by the next generation of accelerators," explains Markus Körfer, head of the Service Centre Accelerators and Experiment Setup at DESY.

Simone Andresen in front of the prototype, holding a model of the girder she designed

Picture: DESY, Christian Schmid

Accurate to within a micrometre

PETRA IV will replace PETRA III, and to do so the existing storage ring X-ray source is to undergo an extensive conversion. The present facility is itself one of the most powerful of its kind in the world and is used by research and industry to conduct experiments, for example in materials science. Its electron beam produces extremely brilliant X-rays, which the researchers shine at their samples at various experimental stations connected to the facility. "PETRA IV will extend the range of X-ray vision to all length scales, from millimetres down to individual atoms," says Wim Leemans, Director of DESY's Accelerator Division. "This will allow research teams to analyse processes inside a catalytic converter, a battery or a microchip under realistic operating conditions with even greater precision than before and to specifically tailor materials with nanostructures or even active ingredients for medicines."

"PETRA IV will extend the range of X-ray vision to all length scales, from millimetres down to individual atoms"

Wim Leemans, DESY

To achieve this, however, the electron beam travelling round the 2.3-kilometre-long circular tunnel must be held on its path with even greater precision. And that is quite a challenge: Massive as the frames supporting the conducting magnets may be, they do vibrate. External drivers, such as the pumps for the water cooling system or heavy traffic in the area, can cause the girders to vibrate minimally. This is unavoidable and can be tolerated to a certain extent. Problems arise when the frequency of the external excitation corresponds to the natural frequency of the girders, leading to resonance. What happens then is, in principle, the same as ›› when parents push their child on a swing: If their pushes are timed to be in the right rhythm, the child will swing higher and higher.

"In a synchrotron radiation source, however, it is essential to prevent oscillations from building up in this way," explains Riccardo Bartolini, project manager for the PETRA IV accelerator. "The PETRA IV beam should not deviate from its optimal trajectory by more than 100 nanometres, that is one ten-thousandth of a millimetre." To achieve this, the components must be positioned and aligned to within a few micrometres (thousandths of a millimetre). Above all, the natural frequency of the magnet support frames must not be too low: "Anything with a natural frequency below 26 hertz risks resonating with external excitations," says Daniel Thoden, an expert in mechanical engineering from Körfer's group.

"The PETRA IV beam should not deviate from its optimal trajectory by more than 100 nanometres"

Riccardo Bartolini, DESY

Lightweight solution

In this case, since the external drivers are a given, it is necessary to modify the natural frequency of the system itself, the rhythm with which it oscillates, to prevent resonance from occurring. For the child on the swing, this could perhaps involve changing the length of the ropes – for PETRA IV, the experts are adjusting the vibrational properties of the support frames. This cannot be achieved by making them even more massive, however. That would make the girders too heavy and too expensive. Instead, a stable lightweight solution with a high frequency of oscillation was required. To identify it, DESY's physicists entered into an unusual alliance: with marine biologists.

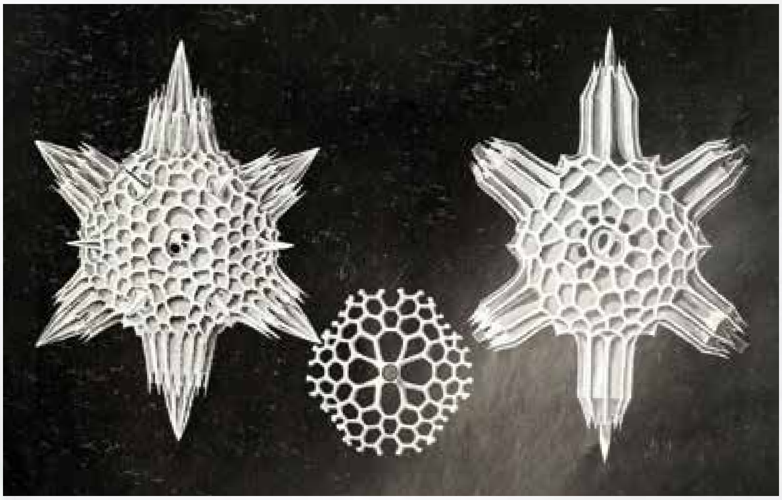
The Alfred Wegener Institute, or AWI for short, Helmholtz Centre for Polar and Marine Research in Bremerhaven, not only studies the oceans, life in them and how climate change is affecting it. The Bionic Lightweight Optimisation and Functional Morphology team, led by Christian Hamm, has been successfully applying findings from the maritime world to industry and technology for many years. The key word here is bionics: using nature as a model for technical applications.

Marine biologist Simone Andresen stress testing the prototype with Normann Koldrack (l.), head of the girder work package of DESY's PETRA IV project, and DESY's vibration expert Norbert Meyners (r.)

Picture: DESY, Christian Schmid

Through the transfer departments of the two Helmholtz centres, the physicists at DESY have now cooperated with the biologists and engineers at AWI to develop novel support frames inspired by nature. To meet the requirements imposed by accelerator physics, Simone Andresen, project leader and doctoral student at AWI, looked around in nature for a construction principle that is both stable and lightweight and oscillates at the highest possible frequency. She found what she was looking for in the aforementioned radiolarians and the similarly built and equally tiny diatoms. The silicate shells of both are almost impossible for predators such as copepods to crack. Yet they are so light that the micro-organisms can float right up near the surface of the sea. And this despite the fact that silicate is significantly more dense than water.

Example of the filigree shapes of radiolarians, captured by the naturalist Ernst Haeckel in his book "Art Forms of Nature" (1904)



"It looks chaotic. But especially when the applied loads are not uniformly distributed, an irregular structure is the most stable."

Simone Andresen, AWI

Mixture of honeycomb and spider's web

The tiny creatures achieve the desired combination of rigidity and lightness through the fine branching and the struts in their corset. "In detailed analyses, we have determined that these are only attached at sites where there are actually external forces to be absorbed," explains Andresen. "This is the same reason why you only need four thin table legs to hold up a kitchen table along with everything on it. It's stable – but of course it requires much less material and is much lighter than if the tabletop was resting on a solid block of wood." In addition, the struts have rounded angles where they join. This contributes to their strength as well.

Andresen used a computer to model how the load paths within such a structure unfold under different conditions. She then designed a prototype based on her findings. What is particularly striking about the new assembly is the substructure, which resembles a mixture between a honeycomb and an irregular spider's web. "It looks chaotic. But that is one of the key findings of the project: Especially when the applied loads are not uniformly distributed, an irregular structure is the most stable if it is to be lightweight at the same time."

The prototype is made of cast iron. In initial load tests, its vibrations were indeed close to those calculated by the computer. "We have now completed the concept phase and demonstrated that it works," says Daniel Thoden. "But the design phase is yet to come."

From research to building bridges

The prototype itself is unlikely to be used in its present form because the magnet optics of PETRA IV are being developed in parallel, and they will have a major influence on the final product. Realistically, though, a kind of hybrid between conventional and new construction principles could be used that meets the vibrational criteria while requiring as little material as possible.

Andresen's prototype will hence serve as a reference that will inspire the at least partially novel design of the next girder generation. However, the application of this technology, jointly developed by DESY and AWI, will not stop there. Even beyond PETRA IV, many applications call for low-vibration, lightweight constructions modelled on nature – for example, for the frames supporting lasers and other precision instruments used in research. And, of course, wherever vibrations need to be prevented in complex structures, from industrial production lines to bridges.

The oldest skeletons of radiolarians have been found in Australia, dating back to the Middle Cambrian, which makes them more than 500 million years old. In the future too, their ancient ingenious design principle will be widely imitated – not least in high-tech research.

Quantum physics in proteins

Artificial intelligence affords unprecedented insights into how biomolecules work

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

A new analytical technique is able to provide hitherto unattainable insights into the extremely rapid dynamics of biomolecules. The developers, led by Abbas Ourmazd from the University of Wisconsin–Milwaukee and Robin Santra from DESY, used a clever combination of quantum physics and molecular biology to track the way in which the photoactive yellow protein (PYP) undergoes changes in its structure in less than a trillionth of a second after being excited by light.

"In order to precisely understand biochemical processes in nature, such as photosynthesis in certain bacteria, it is important to know the detailed sequence of events," Santra explains the underlying motivation. "When light strikes photoactive proteins, their spatial structure is altered, and this structural change determines what role a protein takes on in nature." Until now, however, it has been almost impossible to track the exact sequence in which structural changes occur. Only the initial and final states of a molecule before and after a reaction can be determined and interpreted in theoretical terms. "But we don't know exactly how the energy and shape changes in between the two," says Santra. "It's like seeing that someone has folded their hands, but you can't see them interlacing their fingers to do so."

"It's like seeing that someone has folded their hands, but you can't see them interlacing their fingers to do so"

Robin Santra, DESY

Whereas a hand is large enough and the movement is slow enough for us to follow it with our eyes, things are not that easy when looking at molecules. The energy state of a molecule can be determined with great precision using spectroscopy; and bright X-rays, for example from an X-ray laser, can be used to analyse the shape of a molecule. The extremely short wavelength of X-rays means that they can be used to resolve very small spatial structures, such as the positions of the atoms within a molecule. However, the result is not an image like a photograph, but instead a characteristic diffraction pattern of the X-rays, which can be used to deduce the spatial structure that created it.

Bright and short X-ray flashes

Since the movements are extremely rapid at the molecular level, the scientists have to use extremely short X-ray pulses to prevent the image from being blurred. It was only with the advent of X-ray lasers that it became possible to produce sufficiently bright and short X-ray pulses to capture these dynamics. However, since molecular dynamics takes place in the realm of quantum physics where the laws of physics deviate from our everyday experience, the measurements can only be interpreted with the help of a quantum-physical analysis.

There is one special feature of photoactive proteins that needs to be taken into account: The incident light induces their electron shell to enter an excited quantum state, and this causes an initial change in the shape of the molecule. This change in shape can in turn result in the excited and ground quantum states overlapping each other. In the resulting quantum jump, the excited state reverts to the ground state, whereby the new shape of the molecule initially remains unchanged. The conical intersection between the quantum states therefore opens a pathway to a new spatial structure of the protein in the quantum-mechanical ground state.

The team led by Santra and Ourmazd has now succeeded for the first time in unravelling the structural dynamics of a photoactive protein at such a conical intersection. They did so by drawing on machine learning, because a full description of the dynamics would in fact require every possible movement of all the particles involved to be considered. This quickly leads to unmanageable calculations that can no longer be solved.

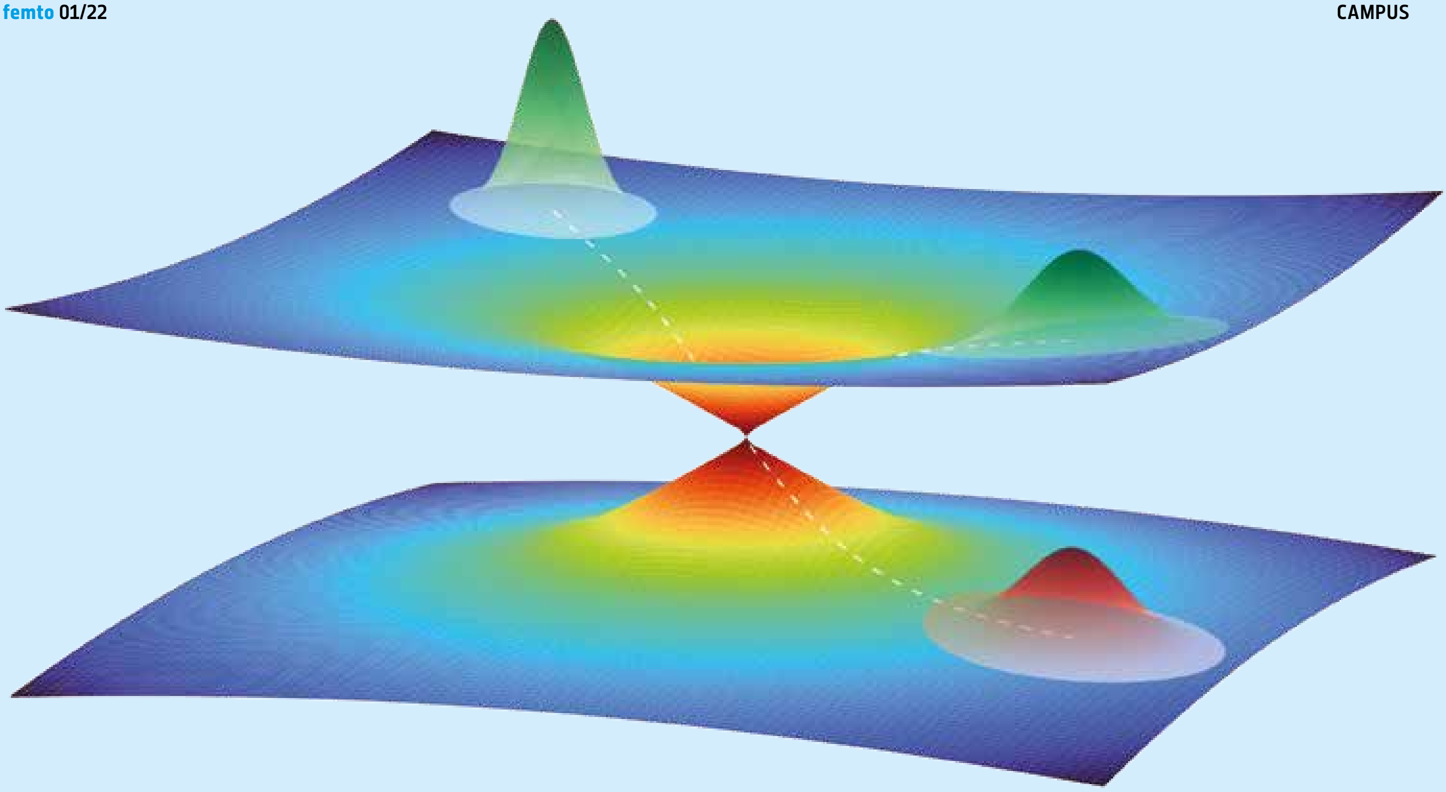


Illustration of a quantum wave packet in close vicinity of a conical intersection between two quantum states. The wave packet represents the collective motion of multiple atoms in the photoactive yellow protein. A part of the wave packet moves through the intersection from one potential energy surface to the other, while the other part remains on the top surface, leading to a superposition of the two quantum states.

6000 dimensions

"The photoactive yellow protein we studied consists of some 2000 atoms," explains Santra, who is a lead scientist at DESY and a professor of physics at Universität Hamburg. "Since every atom is basically free to move in all three spatial dimensions, there are a total of 6000 options for movement. That leads to a quantum-mechanical equation with 6000 dimensions – which even the most powerful computers today are unable to solve."

However, computer analyses based on machine learning were able to identify patterns in the collective movement of the atoms in the complex molecule. "It's like when a hand moves: There, too, we don't look at each atom individually, but at their collective movement," explains Santra. Unlike a hand, where the possibilities for collective movement are obvious, these options are not as easy to identify in the atoms of a molecule. However, using this technique, the computer was able to reduce the approximately 6000 dimensions to four. By demonstrating the new method, Santra's team was also able to characterise a conical intersection of quantum states in a complex molecule made up of thousands of atoms for the first time.

The detailed calculation shows how this conical intersection forms in the four-dimensional space and how, after being excited by light, the photoactive yellow protein changes its shape while dropping back through the intersection to its initial quantum state. The scientists can now describe this process in steps of a few dozen femtoseconds (quadrillionths of a second) and thus advance the understanding of the photoactive processes. "As a result, quantum physics is providing new insights into a biological system, and biology is providing new ideas for quantum-mechanical methodology," says Santra, who is also a member of the Hamburg cluster of excellence "CUI: Advanced Imaging of Matter". "The two fields are cross-fertilising each other in the process."

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Picture: DESY, Niels Breckwoldt

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The DESY research centre

DESY is one of the world's leading particle accelerator centres and investigates the structure and function of matter – from the interaction of tiny elementary particles and the behaviour of novel nanomaterials and vital biomolecules to the great mysteries of the universe. The particle accelerators and detectors that DESY develops and builds at its locations in Hamburg and Zeuthen are unique research tools. They generate the most intense X-ray radiation in the world, accelerate particles to record energies and open up new windows onto the universe.

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