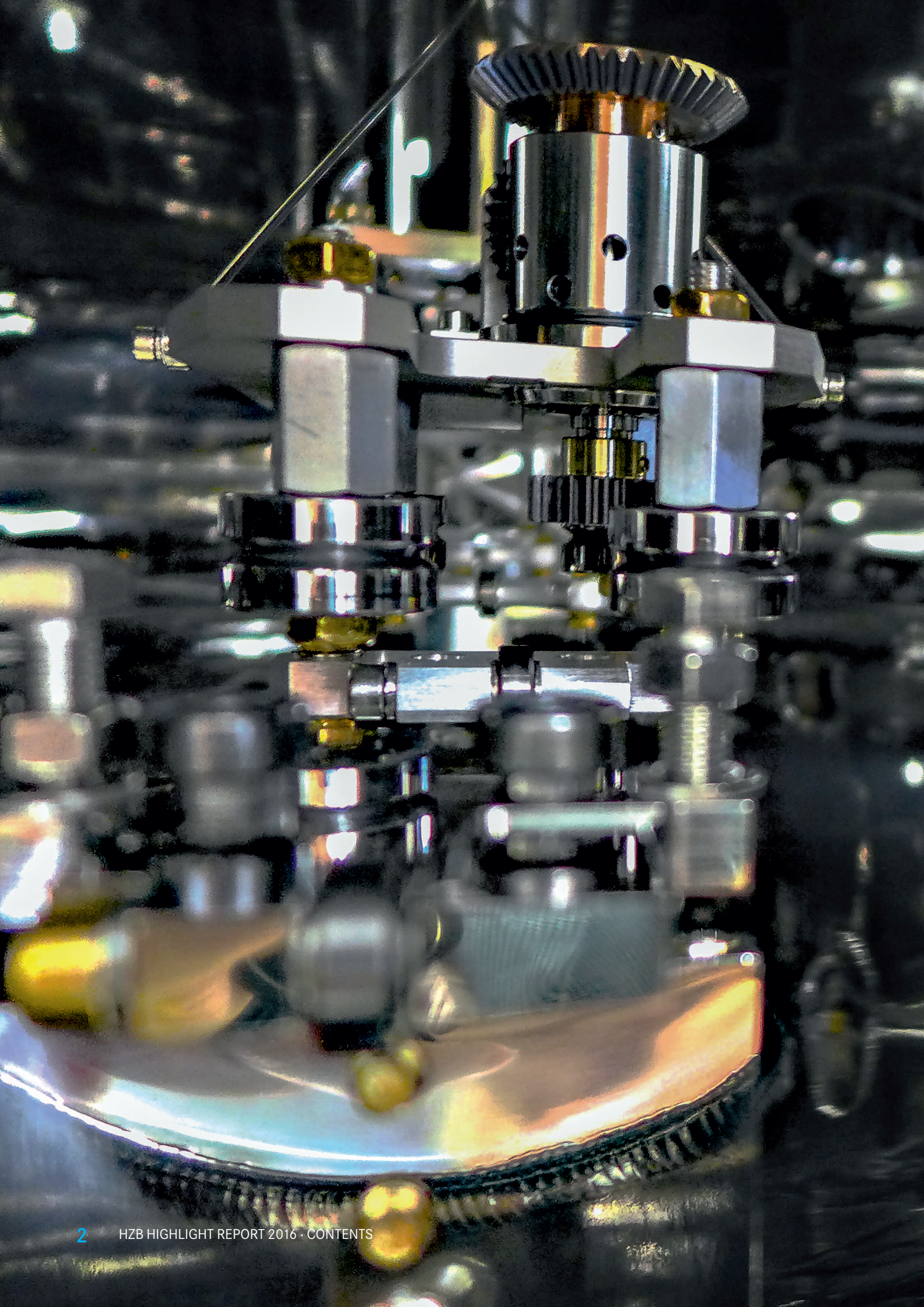
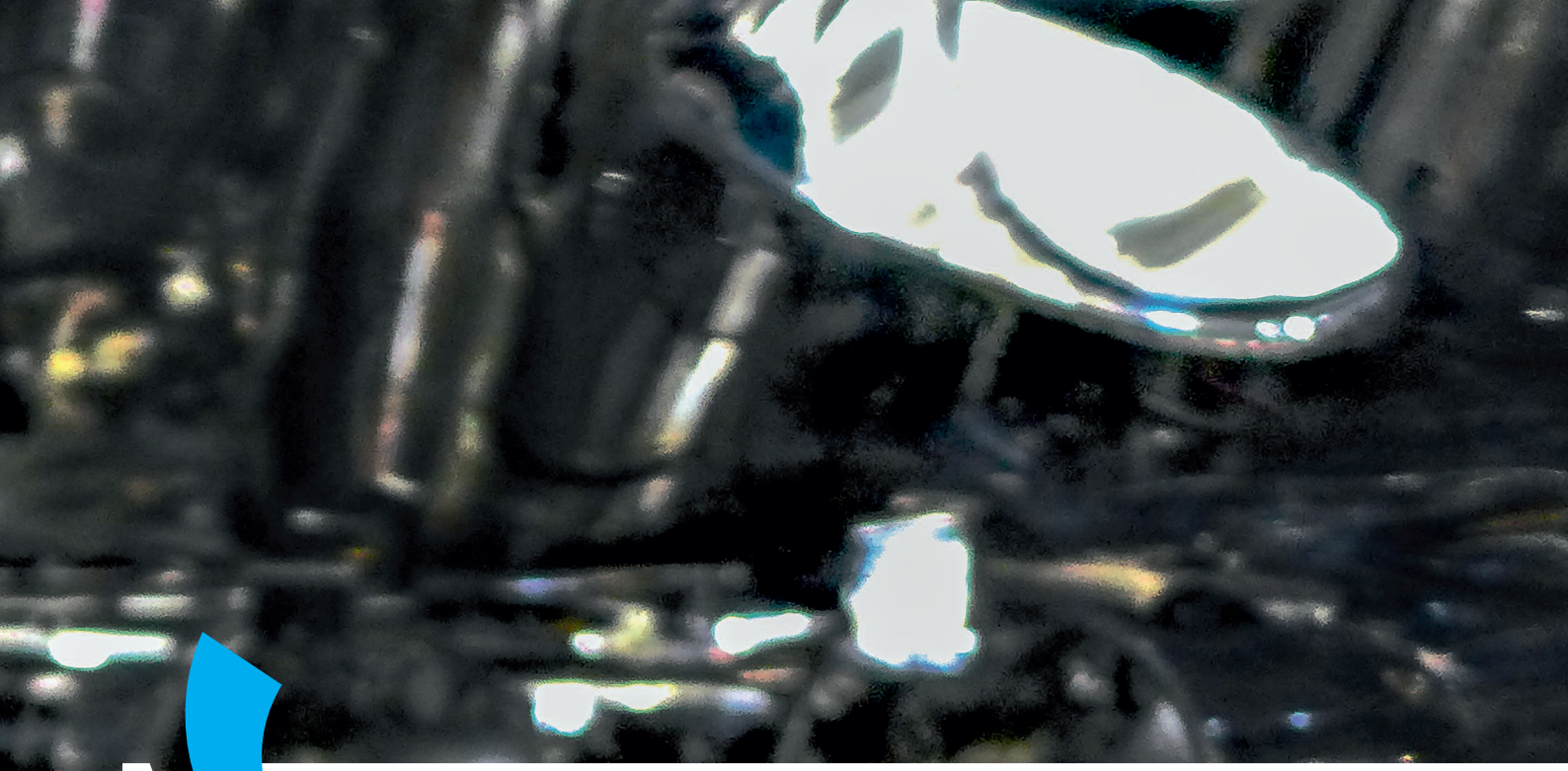
HZB Helmholtz Zentrum Berlin

FOCUSSING ENERGY REALISING VISIONS

HIGHLIGHTS 2016

Research highlights at the Helmholtz-Zentrum Berlin für Materialien und Energie





CONTENTS

AN OUTCOME THAT'S PLAIN TO SEE

2016 was an eventful year for Helmholtz-Zentrum Berlin: In October, the laboratory complex EMIL@BESSY II (Energy Materials In situ Laboratory) in Adlershof was inaugurated in the presence of the Federal Minister for Research, Johanna Wanka; in Wannsee, HZB began construction of a new laboratory building for energy materials. These two events exemplify how, after successfully concluding its two-year strategy process, HZB is continuing to invest in expanding the infrastructure it needs. This commitment is key to continuing to achieve top level research results in future and to strengthening the profile of HZB.

An online survey we conducted at the beginning of this year reveals the overall awareness of the course we have chosen. Two thirds of those surveyed are familiar with HZB's research profile. For example, 64 per cent know that we are researching energy materials, 61 per cent are aware of our photovoltaics research, and 58 per cent know that HZB is a place for researching with synchrotron radiation. 48 per cent also named research with neutrons as a topic at HZB.

This Highlight Report 2016 presents results from all of these thematic areas. And, of course, we once again present examples of how fruitfully the users work at the research infrastructures we operate, BESSY II and BER II.

Prof. Dr. Bernd Rech and Thomas Frederking.

A challenge over the past few years has been guaranteeing we can go ahead with the upgrade of our synchrotron radiation source BESSY II into the variable-pulse-length storage ring BESSY-VSR. This strategic prioritisation, which was decided in the strategy paper in 2015 and is supported by all internal and external bodies, received a financial commitment in 2017. These are the fruits of the efforts of all parties involved at HZB, in research and administration, and important proof of our funders' belief in Berlin as a centre for research with soft X-rays. In this Highlight Report, you can read how it took many small steps to achieve this success. Scientific curiosity, brilliant ideas, and decades of experience in the development and operation of the synchrotron source have all neatly converged to be seen as one at this strategically favourable moment.

From this, we see that scientific freedom and strategic foresight must go hand in hand if a major research centre like HZB wishes to be successful. The merit for reconciling these two aspects so effectively over the past years goes to Prof. Dr. Anke Kaysser-Pyzalla, the scientific director of HZB from 2009 to 2017. With great perseverance and farsightedness, she accomplished the incredibly demanding task of merging two centres – one from the Leibniz Association, the other from the Helmholtz Association – and their very different cultures into one powerful entity.

Having seen the centre take its present shape, and with its future development set out in the Strategy 2020+, towards the end of last year she decided to apply herself to new tasks. Early in the summer of 2017, Anke Kaysser-Pyzalla

assumed the office of President of the Technische Universität Braunschweig. We wish her all the very best in shaping her new domain.

As you browse through this book, you will notice that HZB is giving fresh impetus to the field of Materials for Future Information Technology.One example is the quantum spin "liquids" studied at HZB, in which electron spins remain mobile even at temperatures very close to absolute zero and which could become components of future quantum computers. HZB is working at the forefront of scientific knowledge in this field. Our activities are primarily in the domain of basic research – but always with a view to real application. It is already foreseeable that these results could have a strong impact on the design of the future computer.

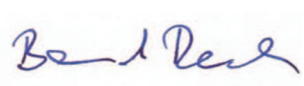
"True to our beginnings, HZB places great importance on research into new photovoltaic materials and solar fuels: this applies both to the advancement of existing systems and to the development of entirely novel material systems."

True to our beginnings, HZB places great importance on research into new photovoltaic materials and solar fuels: this applies both to the advancement of existing systems and to the development of entirely novel material systems, such as perovskite–silicon combinations. This is where two solar cells made from different materials are cleverly combined into one tandem solar cell. Through this, our researchers have brought the efficiencies up significantly higher than would have been possible through independent advancements in these two fields. Perovskites are in fact so promising that, in 2016, HZB decided to establish two new young investigator groups, led by Dr. Steve Albrecht and Dr. Antonio Abate, to reinforce its expertise in this field (page 52). And thanks to our successful application HySPRINT, for "Hybrid Silicon Perovskite Research, Integration & Novel Technologies", we have also boosted technology transfer in this field with funds from the Helmholtz Association.

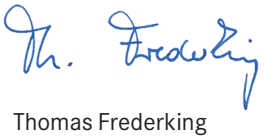
The development of systems for artificial photosynthesis is another topic we have long been pursuing. A team at the HZB institute is hot on the heels of a method that could make the concept truly practicable – where the essential components of the artificial leaf, the electrodes, are not so hasty to self-destruct. This and many other insights shared in our Highlight Report are important stepping stones on the path towards a clean, low-carbon economy.

All of this is only possible because we are continually investing in our research infrastructure at HZB, developing new scientific concepts for this infrastructure, and successfully attracting the necessary funding. At this point, we also mention Dr. Catherine Dubourdieu as one of the brilliant researchers we were able to attract to HZB last year. Since April 2016, she has headed the HZB institute "Functional Oxides for Energy-Efficient Information Technology". With the cover of this book, we welcome her and by extension all of our newly arrived colleagues at HZB.

And now we wish you, our readers, an engaging and informative read. As always, we look forward to receiving your feedback and suggestions on the continuing evolution of our HZB Highlight Report.



Prof. Dr. Bernd Rech
Scientific Director



Thomas Frederking
Administrative Director

GREEN LIGHT FOR BESSY VSR

Since 1998, BESSY II has established itself as the leading source of soft X-rays in Germany and Europe. Unique instruments for analysing energy materials have been installed on nearly 50 beamlines here. Now, its upgrade into BESSY VSR, a variable-pulse-length storage ring, has been approved. The accelerator physicists **Prof. Dr. Andreas Jankowiak** and **Prof. Dr. Jens Knobloch** report on how years of preparation have come together like pieces of a puzzle, and what hurdles have yet to be overcome.

What is so special about BESSY VSR?

AJ: BESSY VSR offers a huge added value for research. For each experiment, a team can choose to study the sample with light pulses of either 15-picosecond or only 1.5-picosecond duration, meaning with over a million pulses per second. Our colleague Alexander Föhlisch and international research groups have identified scientific fields in which BESSY VSR can provide new insights: such as real-time observation of switching processes as they take place inside materials needed for energy-efficient information technology. Or the analysis of chemical processes in solution, or the development of novel catalysts, and many other of our core topics.

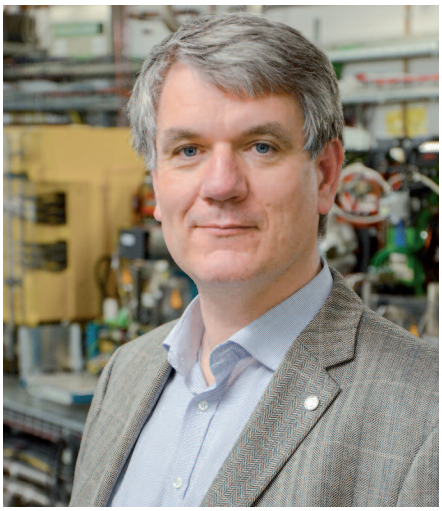
How long have the preparations for BESSY VSR been going on?

JK: Let me just back up first, for a moment. Over the last 15 years or so, we have been taking lots of little steps that now allow us to take the big leap. For example, we started working in 2000 on a concept for a free electron laser (BESSY FEL). It turns out we couldn't implement this concept, but we did learn the trade and even established ourselves as worldwide experts in the process. We built up a test bed for cavities called HoBiCaT, and procured a cryogenic system so that we could develop superconducting cavities. It was only through this groundwork and experience that we could even begin to think about BESSY VSR.

Cavities are very much the key to BESSY VSR: Can you briefly explain what cavities are?

JK: Put simply, cavities are just cylindrical metal housings, inside which standing electromagnetic waves can form, which is why they are also called cavity resonators. All electron bunches circling around the storage ring giving off light pulses, and therefore losing energy, fly through these cavities. As they do so, they are brought back "into shape" (compressed) and recover the lost energy.

AJ: The first concrete idea that superconducting cavities would allow much shorter pulses came from Gode Wüstefeld. He developed this idea together with Jörg Feikes and Peter Kuske and in 2006, put it up for discussion at the EPAC 2006 conference in Edinburgh.



Prof. Dr. Andreas Jankowiak heads up the HZB Institute for Accelerator Physics. The upgrade from BESSY II to BESSY VSR has long been in the planning. The important focus now is the concrete realisation – a task with which HZB will break new ground.

JK: At that time, we had to put it aside and continue working on BESSY FEL. In the end, though, BESSY FEL attracted no funding. But the fact that we had built HoBiCaT allowed us to develop bERLinPro in a very short time, which is a concept for an energy recovery linear accelerator that is now being realised. The miraculous thing is that for the high-current operation of bERLinPro, we have to develop superconducting cavities. Which is exactly what we need for BESSY VSR, too. So, this creates a very welcome synergy.

AJ: Then came the second brilliant idea from Wüstefeld and colleagues that cavities operating at two different frequencies could be built into the one ring. This generates a so-called beating effect, as it is also known in acoustics. This beating causes electron bunches to be compressed to different degrees, allowing many pulses lasting 15 picoseconds to be produced at the same time as pulses ten times shorter in duration. The upshot is that users can choose which pulse duration is best for their experiment.

What do you consider to be the biggest challenges for this project now?

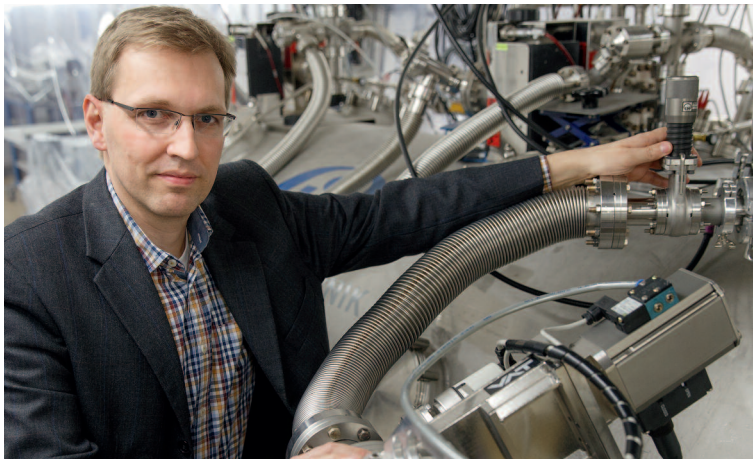
JK: When planning an upgrade for a large facility, usually the goal is to improve a given parameter by an order of magnitude. But the upgrade from BESSY II to BESSY VSR requires a major improvement in not just one parameter, but several. It is truly new territory, and demands a healthy measure of devotion to the task.

AJ: We have four or five arduous, but surely very exciting years ahead of us. We are after all working on a functional storage ring and we have to make sure user operation continues with as little interruption as possible during the conversion.

It was ten years between the first idea and approval of the upgrade. What motivated you to continue pursuing the project for so long?

AJ: The scientific community gave us very strong backing. The Committee for Synchrotron Radiation took a strong stance and said yes, this is the right path for BESSY; the idea must be pursued. Because BESSY VSR can deliver short, high-brilliancy light flashes at a very high repetition rate and thus bridges exactly the gap between the next generation of free electron lasers and synchrotron sources (diffraction limited synchrotrons).

JK: The support from Management was equally essential. They provided the personnel for the development of BESSY VSR before we had any notice of approval. Jobs were created for working out the concept in detail, including the technical design study, all so that BESSY VSR could be approved.



Prof. Dr. Jens Knobloch, head of HZB Institute for SRF Science and Technology.

AJ: In the Technical Design Report, we presented concrete solutions which the scientific community rated as excellent. All synchrotron sources are wondering where we should go from here, and we found our own answer and a project that can be realised. We can all be very proud of that.

JK: It was, and still is, a long march. But now we have a solid foundation: we have the infrastructure and we have the people with the expertise.

Antonia Rötger conducted the interview

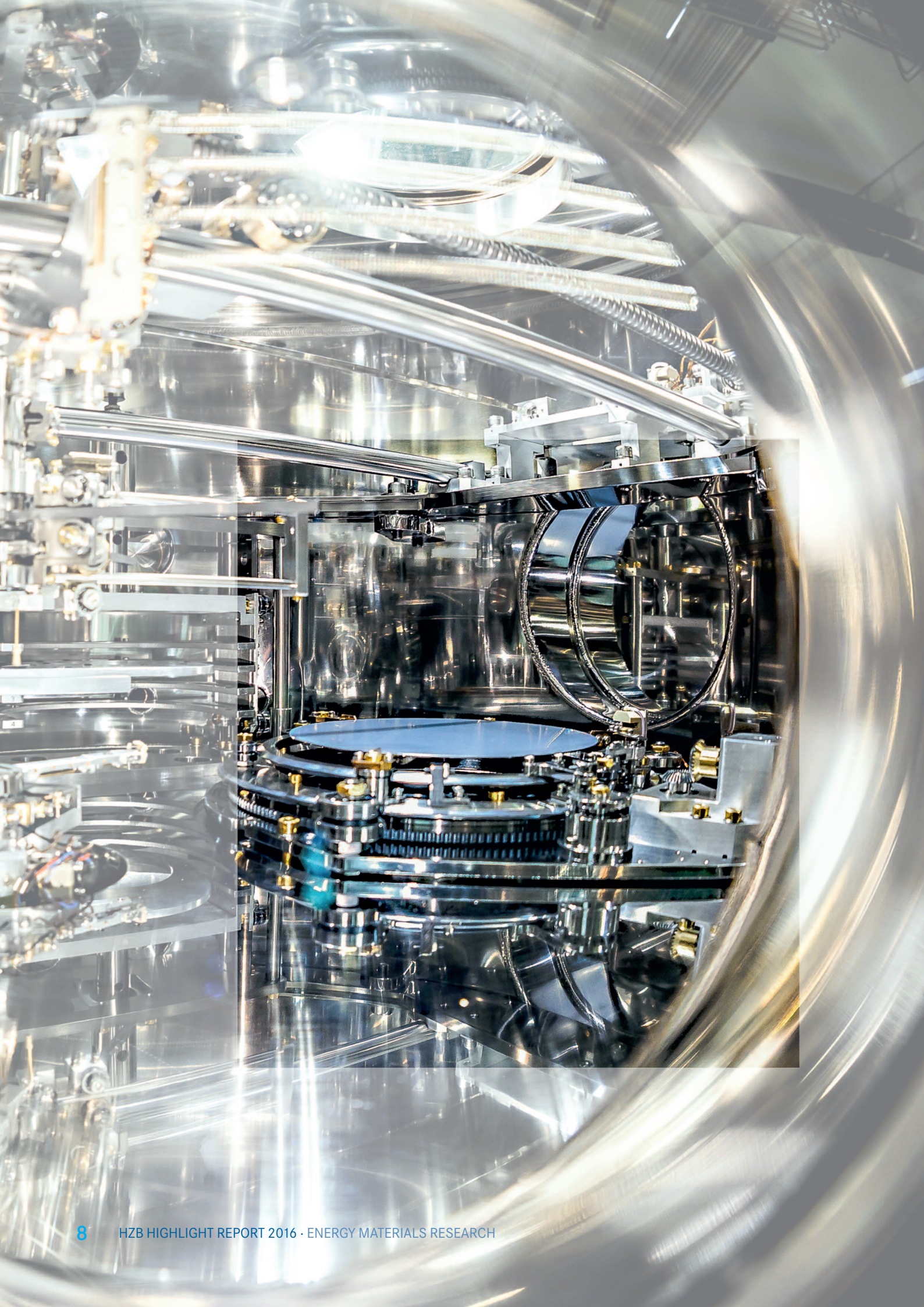
ON THE PULSE OF THE TIMES WITH BESSY VSR

The variable time structure of the light pulses from BESSY VSR (Variable pulse-length Storage Ring) represents an exciting possibility for tackling the core questions of materials research and chemistry. Prof. Dr. Alexander Föhlisch and experts from many fields attended international workshops to figure out where BESSY VSR will allow new insights.

If you need very bright pulses generated with extreme stability to make systematic measurements of material properties, then you can't go past an accelerator-based synchrotron light source. But if you want to investigate extremely fast dynamic processes, you are better off with short-pulse lasers operating in the range of femtoseconds. BESSY VSR is now in the unique process of bringing these two worlds together. BESSY VSR will produce very bright pulses of high stability that additionally possess a time structure for dynamics in the picosecond range. Thus, immediately after performing time-independent experiments, one will be able to observe the functional behaviour of a material or chemical reactions as they unfold. As an example, one will be able to make very precise observations of switching processes inside functional materials. Because these processes are repetitive, to gain a clear understanding of them, we need to characterise the "instantaneous" states at as many points in time as possible. The picosecond pulses from BESSY VSR will be absolutely ideal for this.

The same goes for a chemical reaction. While the whole thing typically kicks off with femtosecond-speed processes inside each molecule, the reaction pathway, which determines the selectivity and reaction rate, continues over a period of picoseconds as atoms rearrange. When it comes to multi-particle systems, a good example would be molecules in solution, which continually collide with one another, transferring energy to or from their neighbouring molecules as they do so. VSR will offer deep new insights into these types of kinetics in realistic systems. With BESSY VSR, we have embarked on a scientific and technological journey that we are sure many will be closely watching. We can proudly say that, with this development, we have cemented our leading position in the field of research using soft X-rays. The funding is proof of our funders' belief in the innovative power of Berlin. The message is: developments are happening here in Germany that will propel us forward internationally.

Alexander Föhlisch



ENERGY MATERIALS RESEARCH

After three years of construction, the **Energy Materials In-Situ Laboratory (EMIL)** was fully completed in October 2016. At the new laboratory complex, which offers direct access to the brilliant light of the electron storage ring BESSY II, researchers are looking to synthesise and analyse materials for future renewable energy generation. Around 20 million euros were invested in the construction of the laboratory.

In May 2016, HZB procured 800,000 euros in funding for its project **"Atmospheric Cost-Competitive Elemental Sulpho-Selenisation for CIGS" (ACCESS-CIGS)**. In this project, the manufacturing process for CIGS thin-film solar cells will be further optimised together with partners from Germany and the Netherlands. The process developed at the Photovoltaics Competence Centre Berlin (PVcomB) requires no vacuum, involves no toxic gases, and is becoming steadily cheaper. Funding is being provided by the SOLAR-ERA.NET Initiative.

HZB is a member of the **Alliance BIPV (Allianz Bauwerk-integrierte Photovoltaik)**, founded in April 2016. Members of the Alliance BIPV include renowned companies, institutions and experts from the construction industry, electrical engineering and the energy sector. In addition to manufacturers, architects and planners, research institutions, technical inspectors and consultants participate in the Alliance BIPV. Thus, the Alliance BIPV also sees itself as a think tank for building-integrated photovoltaics.

HZB was involved in the **"White Paper for CIGS Thin Film Solar Cell Technology"** published by industrial companies and research institutes. 30 renowned, international CIGS experts, including Prof. Dr. Rutger Schlatmann and Prof. Dr.-Ing. Hans-Werner Schock from HZB, have come to the clear conclusion that it is still worthwhile for property owners to invest in a solar power system employing CIGS thin-film technology.

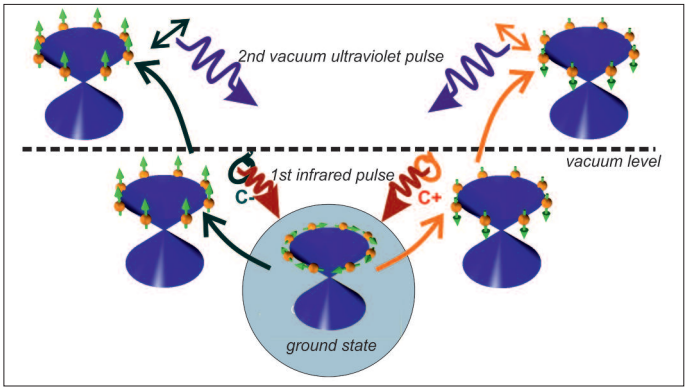
NEW DEVELOPMENTS IN SPINTRONICS

Future information technologies should employ considerably less energy for processing data and provide an **increased data density** as well. Scientists at HZB have approached these goals with different materials and methods.

Topological insulators constitute an exciting class of materials for data storage. They are distinguished by their electrons at the surface being extremely mobile, while the bulk material within is an insulator and does not conduct. Since electrons also simultaneously carry a magnetic moment (spin), topological insulators might also make "spintronic" components feasible. Spintronic components would not be based on the movement of charge carriers such as electrons (as in semiconductor components), but instead on the transport or manipulation of their spins. This would require considerably less energy.
An international team headed by HZB physicist Dr. Jaime Sánchez-Barriga has now shown how the spins of the electrons in topological insulators can be controlled. The team was made up of experimentalists from the Max Born Institute in Berlin and Lomonossow University Moscow, together with theoreticians from Ludwig-Maximilians-Universität München (LMU). The scientists investigated samples of antimony-telluride, a topological insulator, using circularly polarised laser light. They were able to initiate and direct currents of electrons whose spins were oriented in parallel (i. e. spin-polarised currents) using the "rotational direction" of the laser light. In addition, they were successful in changing the orientation of the spins as well.
"If you were to utilise magnetically doped topological insulators, you could also probably store this spin information", explains Ass. Prof. Dr. Oliver Rader, who heads the research group for green spintronics at HZB. "To investigate this, however, and also be able to explore the dynamic behaviour of the magnetic moments in particular, ultra-short light pulses in the soft X-ray region are needed. These kinds of experiments can become standard with the planned upgrade of the BESSY II synchrotron source to BESSY-VSR", he hopes.

Graphene on silicon carbide could be a candidate for spintronics

The realisation of applications for future spintronics requires the development of materials that can conserve the spin information over long distances and also manipulate it.



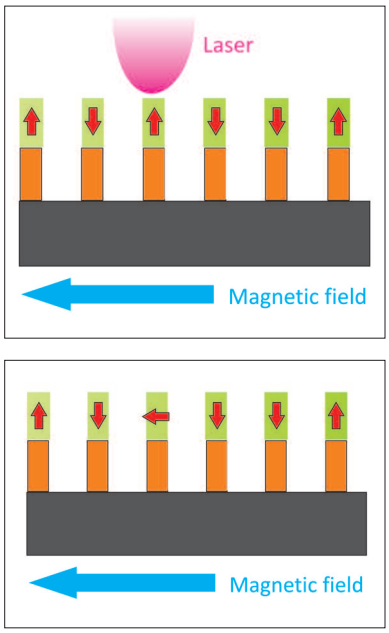
The illustration depicts the characteristic spin orientation (arrows) of electrons in a topological insulator (below). Using an initial circular polarised laser pulse, the spins are excited and point up or down. This can be proven by a second linearly polarised laser pulse (above).

In this context, graphene, a modification of carbon, has been discussed because of the long distances the electron spin can travel without losing its orientation. A couple of years ago, HZB researchers Dr. Andrei Varykhalov and Dr. Dmitry Marchenko demonstrated that also the complete opposite is possible with graphene. Graphene rotates the spin of the electrons when brought in close contact with gold atoms.
This finding has led to a number of breakthroughs in the meantime. They had, however, a common disadvantage. In order to get the gold atoms really close to the graphene, graphene was deposited on a metal substrate such as nickel, and the gold could afterwards easily be squeezed between the graphene and the metal. This enhanced the so-called spin-orbit interaction in the material by a factor of 10 000. Calculations show that an effect of this order of magnitude is linked to a half-rotation (180°) of spins after travelling about 40 nanometres. This is the length scale where miniaturisation of conventional electronic devices has arrived nowadays. Because the substrate is a bulk metal and conducting, there are many more electrons flowing with completely random spin orientation which causes

something like a short-circuit to the spin information. This means that the graphene has to be grown on an insulating substrate. The semiconductor silicon carbide is a famous substrate for graphene. The difficult task was to control the charge doping of the sample. Interestingly for small amounts of gold, the graphene charges negatively and for larger amounts it reverses and charges positively. Marchenko, who had employed the trick with the gold on the nickel in his Ph. D. thesis, recalls that "it was very difficult to produce the pure positively charged phase". After many trials he succeeded and could study it with the method of spin-resolved photoelectron spectroscopy. What Marchenko found was a very different behaviour as compared to graphene on previous, bulk metallic, substrates. He searched for large spin-orbit effects near hybridisation points, so-called hot spots in the band dispersion. He found there a very large splitting of 100 meV, in the same enhancement by 10,000 over pure graphene. However, the effect is only limited to the vicinity of the hot spot. For the researchers this means that to make use of the high spin-orbit effects of graphene on semiconductors, they need to dope the system by a second element or use a gate voltage to move the hot spot to the Fermi energy where it can contribute to the transport. "In this case, a rather small gate voltage change should modify the splitting from 0 to 100 meV, working as an on/off switch for spin effects in a graphene-based device", Marchenko says.

Efficient material system for Heat-Assisted Magnetic Recording

To increase data density further in storage media, the industry is searching for materials systems with stable magnetic domains on the nanoscale. For overwriting a specific nanoscopic region with new information, a laser is used to heat locally the bit to approximately the so-called Curie-temperature, typically several hundred degrees Celsius. Upon cooling, the magnetic domain in this region can be re-oriented in a small external magnetic field, known as Heat-Assisted Magnetic Recording (HAMR). In industry, iron-platinum materials are currently used as magnetic media for the development of such HAMR-data storage devices. Dr. Jaime Sánchez-Barriga and his team has now examined a new storage media system of dysprosium and cobalt which shows key advantages with respect to conventional HAMR materials: A much lower writing temperature, a higher stability of the magnetic bits, and a versatile control of the spin orientation within individual magnetic bits. They achieved this by sputtering a thin film of dysprosium and cobalt onto a nanostructured membrane. The membrane was produced by scientific cooperation partners at the Institute of Materials Science of Madrid. The system shows a honeycomb antidot pattern with distances of 105 nanometres between nanoholes, which are 68 nanometres in diameter. These nanoholes themselves act as pinning centres for stabilising magnetic wall displacements. The magnetic moments of $DyCo_5$ are perpendicular to the plane and stable against external magnetic fields.



A thin film of dysprosium-cobalt (green) has been sputtered on top of the membrane, resulting in an array of antidots. The magnetic moments of $DyCo_5$ are perpendicular to the plane and stable against external magnetic fields. A laser pulse can be used to locally increase the temperature of individual bits. Moderate heating up to 80° Celsius tilts the magnetic moment associated to a single bit into the plane. Upon cooling to room temperature, the magnetic moment stays in plane until it is overwritten by a magnetic writing head.

The scientists could demonstrate that warming the system to only 80 degrees Celsius is sufficient to tilt the magnetic moments in the $DyCo_5$ film parallel to the surface plane. With measurements at the PEEM and XMCD instruments at BESSY II, they could map precisely the magnetic signals before, during and after warming. After cooling to room temperature, it is then easy to reorient the magnetic domains with a writing head and to encode new information. "This process in $DyCo_5$ is energy-efficient and very fast", states Dr. Florin Radu, co-author of the study. "Our results show that there are alternative candidates for ultrahigh density HAMR storage systems which need less energy and promise other important advantages as well", adds Sánchez-Barriga.

arö

Phys. Rev. B 93, 155426 (DOI: 10.1103/PhysRevB.93.155426): Ultrafast spin-polarization control of Dirac fermions in topological insulators; J. Sánchez-Barriga, E. Golias, A. Varykhalov, J. Braun, L. V. Yashina, R. Schumann, J. Minár, H. Ebert, O. Kornilov, and O. Rader

Appl. Phys. Lett. 108, 172405, 2016 (DOI: 10.1063/1.4947286): Rashba splitting of 100 meV in Au-intercalated graphene on SiC; D. Marchenko, A. Varykhalov, J. Sánchez-Barriga, Th. Seyller, and O. Rader.

Phys. Rev. Applied 5, 064007 (DOI: 10.1103/PhysRevApplied.5.064007): Ferrimagnetic $DyCo_5$ Nanostructures for Bits in Heat-Assisted Magnetic Recording; A. A. Ünal, S. Valencia, F. Radu, D. Marchenko, K. J. Merazzo, M. Vázquez, and J. Sánchez-Barriga

INSCRIBING LOCAL MAGNETIC MONOPOLES

An international collaboration at BESSY II has discovered a new method to inscribe exotic magnetic patterns such as **magnetic monopoles** into thin ferromagnetic films. It might open a new path for the design of energy-efficient data storage.

Magnetic patterns such as monopoles or skyrmions (stable vortices) are promising options for fast and energy-efficient data storage. However, obtaining and manipulating such magnetic structures is not easy. Now, Dr. Sergio Valencia and his colleagues at HZB, in collaboration with the materials science institute of Barcelona, have discovered an interesting new materials system which could do the trick. The samples consisted of regular arrays of superconducting YBaCuO-dots, approximately 20 micrometres in diameter and in different geometries. Valencia and his team covered these microstructures with an extremely thin film of ferromagnetic iron-nickel-alloy, a so-called permalloy.
The experiments were done at low temperatures of 50 Kelvin (minus 223 degrees Celsius), allowing the YBaCuO-dots to be superconducting. To change the magnetic domains inside the permalloy, an external magnetic field, perpendicular to the sample plane, was briefly applied. This external field, not enough to reorient the magnetic domains of permalloy, leads to creation of a so-called supercurrent within the superconducting dots. Such superconducting currents persist even after removal of the external magnetic field and themselves produce a complex magnetic field pattern.
It is this magnetic pattern which rearranges the magnetic domains of the permalloy film on top. It was possible to reorient all domains pointing towards or away from a common centre, similar to magnetic monopoles. Valencia and his colleagues were able to map the magnetic domains of the permalloy by means of X-ray photoelectron emissions microscopy (X-PEEM and XMCD) at BESSY II.
Computer simulations reaffirm how such magnetic patterns are created in the permalloy film via the interaction with the superconducting dots. Choosing different geometries and arrangements of dots can produce and control a multitude of exotic magnetic patterns similar to monopoles as well as skyrmions, a type of stable vortex. “I am quite optimistic that it is possible to miniaturise such patterns to facilitate their implementation in magnetic memories, for example. What is more, we even have some ideas on how to stabilise such magnetic structures at room temperature”, Valencia says. *arö*

Advanced Science, Open Access (DOI: 10.1002/advs.201600207): Encoding Magnetic States in Monopole-Like Configurations Using Superconducting Dots, A. Palau, S. Valencia, N. Del-Valle, C. Navau, M. Cialone, A. Arora, F. Kronast, D. A. Tennant, X. Obradors, A. Sanchez, and T. Puig

CHARGE DENSITY WAVES ARE STEADY IN SPITE OF SUPERCONDUCTIVITY

High-temperature superconductors are special metal oxide materials that pass electrical current without energy losses. In contrast to conventional superconductors that have to be cooled to almost absolute zero, this property appears already at comparably high temperatures. In prototypical yttrium barium copper oxide (YBaCuO), the transition temperature is 92 Kelvin (minus 181 degrees centigrade). Hence, liquid nitrogen suffices as a coolant to reach the superconducting phase. A team of scientists led by Prof. Bernhard Keimer, MPI for Solid State Research, and Dr. Eugen Weschke, HZB, now investigated an artificial layer system composed of alternating nanolayers of YBaCuO and a ferromagnetic material.
As interfaces often determine the properties of such heterostructures, physicists were particularly interested in their role for the present system. During his PhD work using resonant X-ray diffraction at BESSY II, Alex Frano could detect tiny collective modulations of valence electrons around Cu atoms in the YBaCuO layer. Data analysis revealed that the resulting charge density wave does not remain located close to the interface but extends across the whole layer. “This finding is quite a surprise, as previous studies revealed a strong tendency of superconductivity to suppress the formation of charge density waves”, explains Frano.
“Engineering artifical interfaces in heterostructures of ferromagnetic and superconducting layers allowed stabilisation

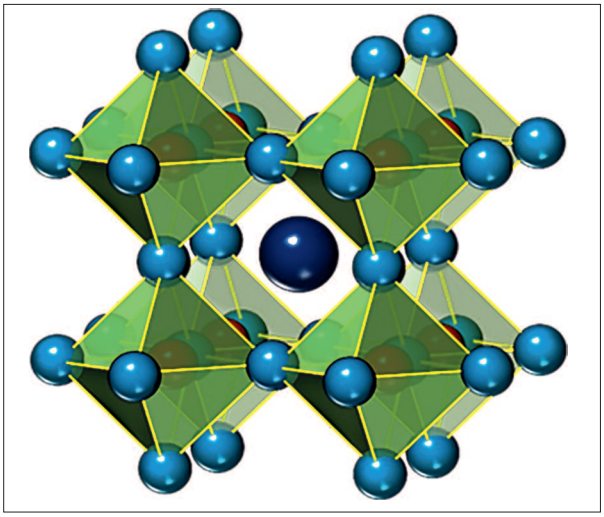
of charge density waves even in the presence of superconductivity: YBaCuO remains superconducting while the charges arrange in a periodic structure", explains Weschke, "exploring the details of this coexistence on a microscopic scale is a challenging task for future experiments." A most exciting perspective of the present results is paving the way to controlling the superconducting state itself. *arö*

Nature Materials 15, 831–834, 2016 (DOI:10.1038/nmat4682): Long-range charge-density-wave proximity effect at cuprate/manganate interfaces, A. Frano, S. Blanco-Canosa, E. Schierle, Y. Lu, M. Wu, M. Bluschke, M. Minola, G. Christiani, H. U. Habermeier, G. Logvenov, Y. Wang, P. A. van Aken, E. Benckiser, E. Weschke, M. Le Tacon and B. Keimer

LASER-INDUCED SWITCHING OF BITS

An international collaboration at BESSY II has demonstrated a completely new approach to overcoming the energy barrier in a magnetic material. This could help to **increase the data density** in future storage media.

The storage capacity of hard disks has increased steadily over the last decades. But now it is approaching limits given by the fundamental laws of physics. Very small magnetic bit-units that can readily be switched by a hard-disk write head tend to become unstable and to lose the stored magnetic information with time. More stable magnetic materials exist but they are so stable that they cannot be switched with the write head any more. Techniques such as heat-assisted magnetic recording overcome this problem by heating the magnetic bit when writing, thereby reducing the energy barrier that needs to be overcome.
An international collaboration has now demonstrated a completely new approach to manipulating the energy barrier in a magnetic material. It lowers the barrier for magnetic manipulation by driving the material across an insulator-to-metal transition. The team led by Prof. Hiroki Wadati from the University of Tokyo studied the material $BaFeO_3$ (BFO) with ultra-short X-ray pulses generated at the Femtospex facility of Helmholtz-Zentrum Berlin. The material is a ferromagnetic insulator with a comparably stable magnetic order. Only when exposed to laser pulses above a certain threshold power does the material turn highly susceptible to an external change of its magnetic state and can easily be switched by an external magnetic field.
By combining magnetic and spectroscopic probe the scientists could identify the threshold for easy magnetisation switching with the formation of a transient metallic state in the material. Unlike in common magnetic materials, where laser-excitation creates a metallic-like state only for less than a trillionth of a second, the electronic structure of BFO leads to a self-stabilisation of this metallic state. It persists about a thousand times longer, bringing the effect in a time range where technical applications become possible. These findings show a new approach to magnetic data manipulation. They also demonstrate the capacity of the Femtospex facility at HZB to combine magnetic and spectroscopic information into a comprehensive picture of ultrafast processes in materials. *red/arö*



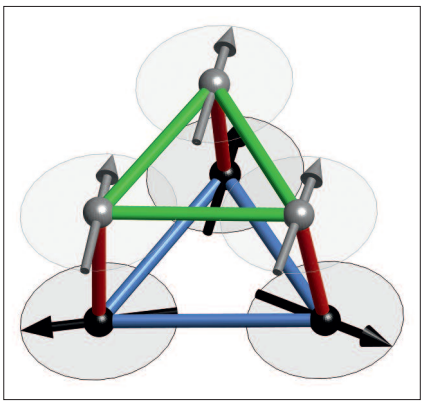
The ferromagnetic material BaFeO3 (BFO) that was shot at with short laser pulses has a perovskite crystal structure.

Phys. Rev. Lett. 116, 256402 (DOI: 10.1103/PhysRevLett.116.256402): Photoinduced Demagnetization and Insulator-to-Metal Transition in Ferromagnetic Insulating $BaFeO_3$ Thin Films. T. Tsuyama, S. Chakraverty, S. Macke, N. Pontius, C. Schüßler-Langeheine, H. Y. Hwang, Y. Tokura, and H. Wadati

OBSERVATION OF A QUANTUM SPIN LIQUID

A novel and rare state of matter known as a **quantum spin liquid** has been empirically demonstrated in a monocrystal of the compound calcium-chromium oxide by a team at HZB. This work deepens our knowledge of condensed matter and might also be important for future developments in quantum information.

Based on our everyday experience, we expect matter to freeze solid at low temperatures with the atoms fixed in a regular arrangement. The magnetic moments arising from the spins of the electrons on the atoms in magnetic materials also come to rest and become rigidly oriented as temperature falls. However, there are some rare exceptions. In what are referred to as quantum spin liquids, the orientations of the electronic spins do not remain fixed even at temperatures near absolute zero.



A section from the crystal lattice of calcium-chromium oxide showing how the spins are subject to conflicting demands. In this ball-and-stick model, the green and red sticks connecting the atoms (grey and black balls) represent ferromagnetic interactions while the blue sticks represent anti-ferromagnetic interactions.

According to conventional understanding, if the interactions are isotropic (where all spin directions are possible), this phenomenon can occur if the spins are arranged in triangular geometries and the interactions between them are antiferromagnetic favouring antiparallel alignment of the spins. For three atoms forming the corners of a triangle, the electronic spin of one atom cannot simultaneously be oriented antiparallel to those on both of the other two atoms. This "frustration" can prevent the spins from coming to rest in a particular orientation even at absolute zero temperature, and instead they move collectively like atoms in a liquid. By contrast, ferromagnetic interactions do not give rise to frustration in isotropic magnets because mutually parallel alignment of the spins can always occur.
For these reasons, only a few isotropic materials have been proposed as spin liquid candidates. Now a team headed by Prof. Dr. Bella Lake has produced and investigated the first monocrystals of calcium-chromium oxide ($Ca_{10}Cr_7O_{28}$). Calcium-chromium oxide is made up of what are known as Kagomé lattices – reminiscent of the pattern of triangles and hexagons woven in Japanese basketry. As a result, a complex set of isotropic magnetic interactions develop in this material consisting not only of anti-ferromagnetic interactions but also much stronger ferromagnetic interactions that according to conventional understanding, should prevent the existence of spin liquid behaviour. However, magnetic and Neutron scattering experiments conducted in Germany, France, England and the USA, as well as muon spectroscopy experiments performed at the Paul-Scherrer-Institute in Switzerland have shown that the spins in these samples retain their collective motion even at temperatures as low as 20 millikelvin and behave like a quantum spin liquid.

More candidates for spin liquids expected

Theoretical physicist Prof. Johannes Reuther of HZB has now been able to extend the theoretical model of spin liquids with the help of these experimental clues. He has used numerical simulations to show how the different magnetic interactions in calcium-chromium oxide compete with one another and keep the spins dynamic.
"We have proved empirically that interesting quantum states such as spin liquids can also occur in considerably more complex crystals with different constellations of magnetic interactions", says Dr. Christian Balz, lead author of the work. Lake also explains: "The work expands our understanding of magnetic materials, and also shows us that there are potentially far more candidates for spin liquids than expected. This could be important for the advancement of quantum computers in the future because spin liquids are one of the possible building blocks for carrying the smallest unit of quantum information, known as a qubit." *arö*

Nature Physics 12, 942–949, 2016 (DOI: 10.1038/nphys3826): Physical realization of a quantum spin liquid based on a novel frustration mechanism, C. Balz et. al.

TRAPPED IN A WELL

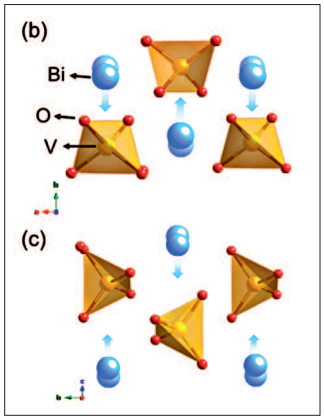
Scientists at HZB have traced the paths taken by charge carriers through a **light-absorbing material** used in hydrogen production. Their insights offer a new way to improve this important process for clean energy generation.

It is an exciting idea in theory – to use sunlight as a power source to split water and then use the resulting hydrogen to make fuels, or use it directly as a fuel itself. In practice, however, the technology has run up against an obstacle that can only be overcome once the exact paths taken by electric charge carriers generated inside a solar energy material are known. HZB researcher Dr. Rainer Eichberger is using ultra-short laser flashes to study exactly these paths.

We can already exploit sunlight to convert water into its constituent elements hydrogen and oxygen by using a tandem cell made with materials such as gallium-indium phosphide or gallium-indium arsenide. Problems with these cells, however, are that they only operate at about 14-percent efficiency and the materials are unsuitable for real-world applications because they corrode and thus become useless over time. Alternative tandem cells have been developed using silicon and a coating of bismuth vanadate to split the water. Currently, these barely achieve an efficiency of five percent, which may seem paltry, but bismuth vanadate is already an oxide material, meaning it is essentially already corroded and will therefore remain functional for a lot longer. Developers will be able to improve the properties of this and similar substances considerably once they have learned exactly how the charge carriers propagate through them.

Like a ball resting on a stretched out cloth

An electric charge arises in a semiconductor material when an electron is knocked off its parent atom. As the negatively charged electron travels away, it leaves behind a positively charged atomic core, which the semiconductor researchers simply refer to as a “hole”. The electrons and holes then propagate independently through the crystal and, ideally, reach the outer surface where they can split the water. A problem is that they lose a lot of speed along the way. This loss of speed is attributable to a polarisation that takes place: each electrically negatively charged electron slightly attracts the positive ions in the crystal around it and thereby slightly distorts the lattice. The mutual attraction forces slow the electron down, and a “quasi-particle” is formed out of this electron and the displaced positive ions. “You can liken this process to a ball resting on a stretched out cloth,” Eichberger explains. “Much like the ball makes a small dip, or a well, in the fabric where it rests, an electron or a hole produces a well in the potential. We call this a ‘polaron’.”



In bismuth vanadate, sunlight produces charge carriers that can propagate to the surface of the material, where they can split water into oxygen and the energy carrier hydrogen. Unfortunately, the charge carriers tend to become trapped in “wells”, and can only continue along their path if the natural vibration of the bismuth atoms (blue) and vanadate particles (orange) bumps them out again.

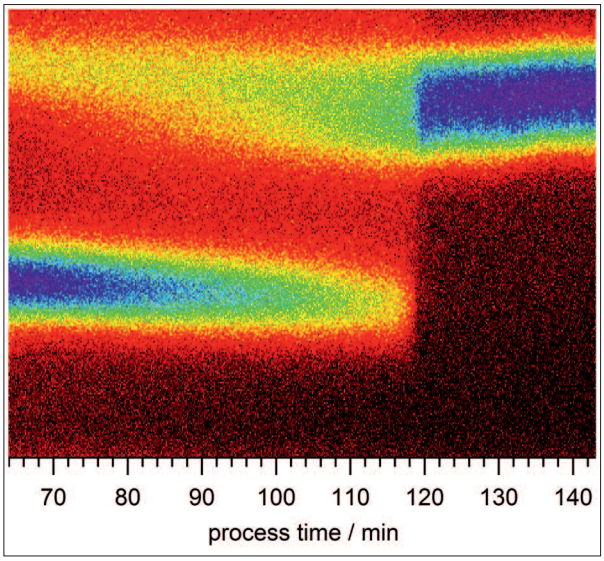
At room temperature, the components of the semiconductor crystal vibrate back and forth and can transfer some of their energy to the polaron, and thus bump the electron out of its well. Using a femtosecond laser, Eichberger has now successfully measured how long it takes for an electron to become trapped in a potential well and, with it, has delivered the first direct evidence of a polaron. The researcher even determined how much energy it takes to bump a charge carrier back out of its well. Eichberger has thus pushed the door open a little further to improving water electrolysis. When researchers know exactly how charge carriers behave, they will be able to search in a targeted manner for materials whose charge carriers intrinsically travel more efficiently to the material surface. In certain cases, they could improve the efficiency of their propagation further still by introducing tiny quantities of other substances that modify the structure of the existing material – a process known as “doping”. *rk*

ACS Energy Letters 2016, 1, 888–894 (DOI: 10.1021/acsenergylett.6b00423): Direct Time-Resolved Observation of Carrier Trapping and Polaron Conductivity in $BiVO_4$; M. Ziwritsch et. al.

HOW DEFECTS APPEAR AND DISAPPEAR IN CIGSE CELLS

An international consortium of scientists has investigated the complex processes during the **deposition of thin chalcopyrite layers**. The scientists were able to observe specific defects as they formed during deposition and under what conditions they self-healed using the BESSY II X-ray source. The results of their research provide clues to optimising fabrication processes.

Copper-indium-gallium-selenide (CIGSe) solar cells have the highest efficiency of polycrystalline thin-film solar cells. The four elements comprising CIGSe are vapour-deposited onto a substrate together to form a very thin layer of tiny chalcopyrite crystals. It is an exceedingly complex process controlled by many variables. This is why CIGSe modules in standard industrial formats have not yet attained the record efficiency already demonstrated at laboratory scale. One possible cause: defects that reduce the efficiency level can form during the course of fabrication. A collaboration of German, Israeli, and British teams has now conducted detailed studies of how different fabrication techniques influence the microstructure. The scientists were able for the first time to observe the defects as they formed during deposition and under what conditions they self-healed by using in-situ X-ray diffraction and fluorescence analysis capabilities at the BESSY II X-ray source.



The data (photon energies over time) show defects (lower signal) which disappear after 120 minutes. This happens at the transition from the copper-poor phase to the copper-rich one.

Improving vapour deposition processes

Vapour deposition of thin CIGSe films is a complex process. Indium, gallium, and selenium are first deposited on the substrate. The deposition of the copper and selenium atoms takes place in a second step. These atoms migrate into the In-Ga-Se layer. Tiny CIGSe crystals of chalcopyrite form there. The concentration of copper only reaches the correct value over the course of this second step. The prior copper-poor phase is characterised by numerous defects within the crystal. The defects increasingly disappear with the addition of copper and selenium. If more copper and selenium atoms are added after reaching the “right” ratio, then these two elements no longer fit into the existing crystal matrix and deposit themselves as copper and selenium grains in and on the polycrystalline CIGSe layer. This is actually problematic, since the grains must be removed afterwards. Nevertheless, they apparently have an important function in reducing the defects to near zero. Dr. Roland Mainz and his colleagues at HZB were able to observe the changes to the film structure during deposition using X-ray diffraction at the EDDI beamline of BESSY II – in realtime. At the same time, they were able to use X-ray fluorescence to analyse the elemental composition of the thin-film layer as it grew. Simultaneous observation with two methods enabled them to obtain a new insight: “The annihilation of the defects takes place very rapidly – just prior to the excess copper-selenium grains being deposited on the surface of the CIGSe film and the film entering the copper-rich phase. So far, we had only understood the copper-rich phase as being important for the growth of the grains. Now we know that it also plays an important role in the elimination of the defects”, explains Mainz.

Temperature is an uncritical parameter

Helena Stange, co-author of the study, simulated the influence of the various types of defects on the diffraction signal. The *in situ* observations fit extremely well with the simulations and with the results derived from different imaging processes used to study the samples in various

stages of deposition by teams at the Max Planck Institute for Solid State Research in Stuttgart, the SuperSTEM Lab in Daresbury, England, and at the Racah Institute in Jerusalem. An additional important result is that the temperature during deposition represents a relatively uncritical parameter for defect elimination. As soon as the layer reaches the copper-rich state, it makes little difference whether the process takes place at 400 degrees Celsius or 530 degrees Celsius. This insight is also of assistance in improving the procedure for depositing onto large surface areas.
The collaboration is part of the Helmholtz Virtual Institute of "Microstructure control for thin-film solar cells" that has been funded since 2012 and ends in 2018. *arö*

Energy Environ. Sci., 2016, 9, 1818-1827 (DOI: DOI: 10.1039/C6EE 00402D): Annihilation of structural defects in chalcogenide absorber films for high-efficiency solar cells; R. Mainz et. al.

A PROTECTIVE LAYER FOR THE "ARTIFICIAL LEAF"

A team at the HZB Institute for Solar Fuels has developed a process for providing sensitive semiconductors for **solar water splitting** with an organic, transparent protective layer. This enhances the efficiency of these so-called artificial leaves considerably.

The "artificial leaf" consists in principle of a solar cell that is combined with further functional layers. These act as electrodes and additionally are coated with catalysts. If the complex system of materials is submerged in water and illuminated, it can decompose water molecules. This causes oxygen and hydrogen to be generated, with the latter storing solar energy in chemical form. There are still several problems with the current state of technology. For one thing, sufficient light must reach the solar cell in order to create the voltage for water splitting – despite the additional layers of material. Moreover, the semiconductor materials that the solar cells are generally made of are unable to withstand the typical acidic conditions for very long. For this reason, the artificial leaf needs a stable protective layer that must be simultaneously transparent and conductive.
The team of HZB worked with samples of silicon, an n-doped semiconductor material that acts as a simple solar cell to produce a voltage when illuminated. Materials scientist Anahita Azarpira, a doctoral student in Dr. Thomas Schedel-Niedrig's group, prepared these samples in such a way that carbon-hydrogen chains on the surface of the silicon were formed. "As a next step, I deposited nanoparticles of ruthenium dioxide, a catalyst," Azarpira explains. This resulted in formation of a conductive and stable polymeric layer only three to four nanometres thick. The reactions in the electrochemical prototype cell were extremely complicated and could only be understood now at HZB.
The ruthenium dioxide particles in this new process were being used twice for the first time. In the first place, they provide for the development of an effective organic protective layer. This enables the process for producing protective layers – normally very complicated – to be greatly simplified. Only then does the catalyst do its "normal job" of accelerating the partitioning of water into oxygen and hydrogen.

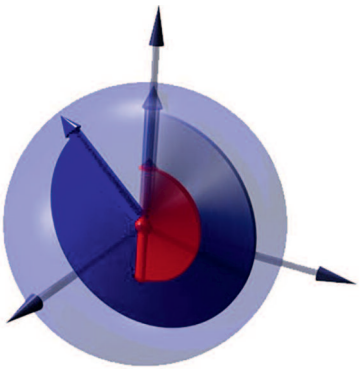
Excellent stability and high current densities

The silicon electrode protected with this layer achieves current densities in excess of 15 mA/cm2. This indicates that the protective layer shows good electronic conductivity, which is by no means trivial for an organic layer. In addition, the researchers observed no degradation of the cell – the yield remained constant over the entire 24-hour measurement period. It is remarkable that an entirely different material has been favoured as an organic protective layer at first: graphene. This two-dimensional material has been the subject of much discussion, yet up to now could only be employed for electrochemical processes with limited success, while the protective layer developed at HZB works quite well. Because the novel material could lend itself for the deposition process as well as for other applications, we are trying to acquire international protected property rights", says Thomas Schedel-Niedrig, head of the group. *arö*

Advanced Energy Materials, Vol. 6, Issue 10, 1502314 (DOI: 10.1002/aenm.201502314): Sustained Water Oxidation by Direct Electrosynthesis of Ultrathin Organic Protection Films on Silicon; A. Azarpira, T. Schedel-Niedrig, H.-J. Lewerenz, and M. Lublow

MORE ENERGY FROM THE SUN BY USING SPINS

Physicists from HZB, Freie Universität Berlin and University of Cambrigde have successfully employed a powerful technique for studying electrons generated through **singlet fission**, a process which it is believed will be the key to more efficient solar energy production in years to come.



Spin, an intrinsic property of electrons, is related to the dynamics of electrons excited as a result of singlet fission – a process which could be used to extract energy in future solar cell technologies.

In most existing solar cells, light particles (or photons) are absorbed by a semiconducting material such as silicon. Each photon stimulates an electron, giving it enough energy to move. In some materials, however, a single photon initially creates one higher-energy, excited particle called a spin singlet exciton. This singlet can form two lower-energy excitons, each with a different spin ("triplet" excitons). For scientists studying how to generate more solar power, it represents a potential bargain – a two-for-one offer on the amount of electrical current generated, relative to the amount of light put in. If materials capable of singlet fission can be integrated into solar cells, it will become possible to generate energy more efficiently from sunlight. But achieving this is far from straightforward. One challenge is that the pairs of triplet excitons only last for a tiny fraction of a second, and must be separated and used before they decay. Their lifespan is connected to their relative "spin", which is an intrinsic angular momentum. Studying and measuring spin through time, from the initial formation of the pairs to their decay, is essential if they are to be harnessed.

A team headed by Prof. Dr. Jan Behrends, junior professor at Freie Universität Berlin and HZB, in cooperation with the University of Cambridge now utilised a method that allows the spin properties of materials to be measured through time. Their experiments have been performed at the Joint EPR Lab, which is jointly funded by HZB and FU Berlin. It provides the opportunity to combine the electron spin resonance (ESR) spectroscopy with other measurement methods. The scientists observed pairs which variously had formed both weakly and strongly linked spin states, reflecting the coexistence of different pairs. Intriguingly, the group found that some pairs which they would have expected to decay very quickly due to their close proximity, actually survived for several microseconds.

Future studies will need to address how to efficiently split the strongly coupled states. Beyond trying to improve photovoltaic technologies, the research also has implications for wider efforts to create fast and efficient electronics using spin, so-called "spintronic" devices. *arö*

Nature Physics 13, 176–181 (DOI: 10.1038/nphys3908): Strongly exchange-coupled triplet pairs in an organic semiconductor; L. R. Weiss et. al.

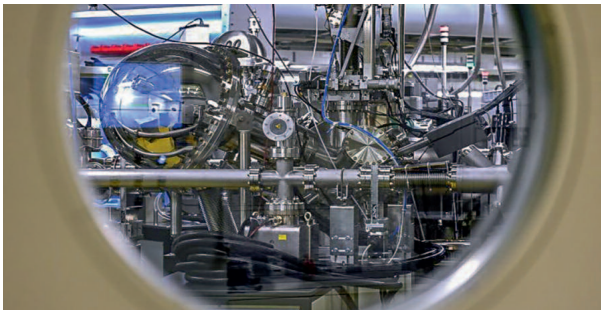
SPEEDING UP CIGS SOLAR CELL MANUFACTURE

A project consortium from research and industry involving the Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin (PVcomB) has been granted a major third-party-funded project called speedCIGS. CIGS solar cells get their name from their constituent elements copper, indium, gallium and selenium. The speedCIGS project will go towards optimising a co-evaporation process at PVcomB used for producing CIGS layers for thin-film solar cells. The manufacturing process used at PVcomB is already being used industrially, but is still relatively slow. The process is now to be sped up within the speedCIGS project, so that more modules can be produced per unit time for the same investment costs. The project is to be funded with 4.7 million euros over four years, of which 1.7 million goes to HZB. *sz/il*

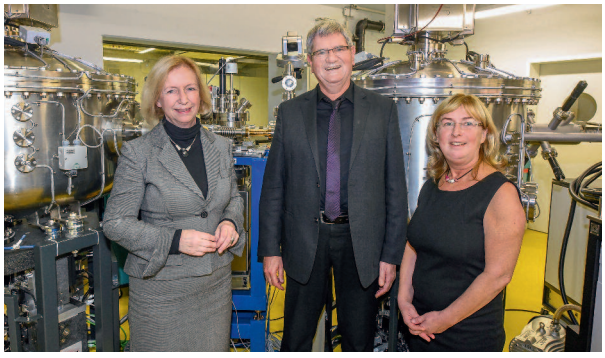
EMIL READY FOR "POWER-TO-X" PROJECT

The German Federal Ministry for Education and Research (BMBF) has created the **"Power-to-X" (P2X) project under its Kopernikus programme**. P2X will advance research in converting electrical energy from the sun and wind into basic chemical compounds, gaseous energy media, and fuels. The HZB will participate in the planned research using its new EMIL laboratory complex.

With its "Kopernikus projects for the energy revolution", the BMBF wants to promote technological and economical solutions for the transition of the energy system. Solar and wind power fluctuate based on seasonal and diurnal cycles as well as on the weather. For that reason, one of the most important requirements for the success of the energy transition is the development of efficient energy storage solutions. One line of funding of the Kopernikus programme is "Power-to-X" (P2X). Its goal is to promote technological advancements that electrochemically convert excess solar and wind power into gaseous energy media, such as hydrogen or into basic chemical compounds. These can then be subsequently stored or processed further into fuels and chemical products. P2X technologies of this kind should make a pivotal contribution to the energy transition. The P2X project is expected to bring new technological developments to industrial maturity within ten years.
The HZB is making available unique means of synthesis and characterisation at its recently launched Energy Materials In-Situ Laboratory (EMIL) in Berlin. The working groups of Prof. Bernd Rech and Prof. Marcus Bär will participate: "We will use the versatile and complementary analytical techniques at the EMIL laboratory to investigate the chemical and electronic properties of catalysts developed by the project partnering organisations," explains Bär, who is coordinating the P2X activities at the HZB. The changes that catalyst materials undergo in electrolytes under realistic conditions will be an important focus of their attention. Simulating real-world operating conditions as closely as possible is vitally important, because catalytically active substances are often only generated under actual operating conditions. Their stability determines the ageing processes and thus the operating life of the electrolyser. "We will further augment the experimental facilities of the EMIL laboratory under the Kopernikus programme in order to facilitate these kinds of "in operando" studies under real atmospheric conditions," Bär elaborates.
A total of 17 research institutions, 26 industrial enterprises, as well as three non-governmental organisations are involved, and the BMBF is funding the first development phase of the project at a level of 30 million euros. Industrial partnering organisations are supplementing the support from the BMBF with research contributions worth an additional 8.3 million euros. P2X will result in the organisation of a research network that incorporates existing large-scale projects and current infrastructure, while expanding connections to industry. The project is being jointly coordinated by RWTH Aachen University, Forschungszentrum Jülich, and DECHEMA. *red*



The new Energy Materials In-Situ Laboratory (EMIL) offers direct access to hard and soft synchrotron X-ray radiation to investigate the chemical and electronic properties of catalysts and other energy materials.

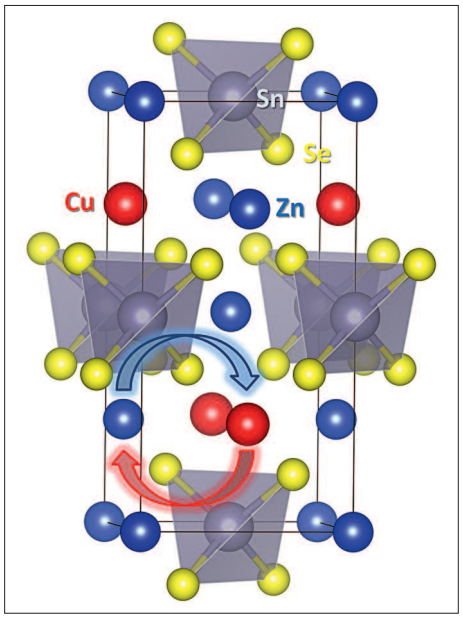


Federal Minister of Research Prof. Johanna Wanka (left) with project managers Prof. Robert Schlögl (MPG) and Prof. Simone Raoux (HZB) at the official inauguration of EMIL on 31 October 2016.

ATOMIC MUSICAL CHAIRS

Researchers at HZB have successfully characterised a striking phase transition in a **kesterite** where the internal structure of the mineral suddenly changes at a given temperature – and have even explained why it happens. This will help in the development of novel solar cells.

The amount of energy that beats down on the earth in the form of sunlight, year after year, is phenomenal: in fact, it exceeds the amount that all of humanity currently uses by about 10,000 times. It is no wonder then that many experts see this inexhaustible source of energy as our future power supply. Until recently, most of our solar electricity has been generated by cells made from silicon. These are easily and reliably manufactured in processes long established in the chip industry, and boast fairly high efficiency in converting the power of the sun to electrical energy. However, the raw material for silicon cells could soon become a bottleneck. Solar cells of the second generation, known as thin-film solar cells, are based on other chemical elements such as indium, gallium, cadmium, arsenic and selenium – yet some of these elements are already quite rare.



The arrangement of copper (red) and zinc (blue) ions within the crystal structure of kesterite is temperature-dependent. The change of positions at rising temperature (blue and red arrows) affects both the electrical and optical properties of the material.

Researchers have therefore been searching for many years for materials that make good alternatives to silicon and other rare elements used in solar cell manufacture. “The so-called kesterites are highly promising for the absorber material in thin-film solar cells,” says Prof. Dr. Susan Schorr, head of the HZB department Structure and Dynamics of Energy Materials. This class of materials is named after the mineral kesterite, a sulphide found in tin deposits, among other places. In addition to sulphur, it contains copper, zinc and tin – elements that are abundant and harmless.
For technical applications that require extremely high purity, the materials are produced artificially. These go by the abbreviated names of CZTS or CZTSe compounds, where the initials stand for copper, zinc, tin and sulphur/selenium. Susan Schorr has been researching such compounds for many years now. The researcher sees numerous advantages in them as photovoltaic materials. “The chemical elements that make up kesterites are available in great abundance – and they include no toxic substances.” There is one problem, however: their efficiency has to be drastically increased if kesterite solar cells are to compete with conventional silicon cells.

Gaining a better understanding of the structure

“We therefore need to understand the crystalline structure and material properties in as much detail as possible,” stresses Dr. Daniel Többens, who researches in Susan Schorr’s team. This is the recent focus of the Berlin scientists’ investigation. Among other things, they have managed to explain a certain effect that was only discovered fairly recently: the arrangement of atoms in kesterite crystals apparently changes below a certain temperature of around 200 degrees Celsius – a striking transition that affects both the electrical and optical characteristics of the material.
“It was already suspected that this effect could be attributed to copper and zinc ions changing their arrangement in the crystalline structure as the material cools down,” says Többens. The team has now directly observed this transition and revealed how the distribution of defects evolves. The transition temperature of the CZTSe material studied at HZB is about 200 degrees Celsius – far below the normal temperature range for manufacturing kesterite thin films

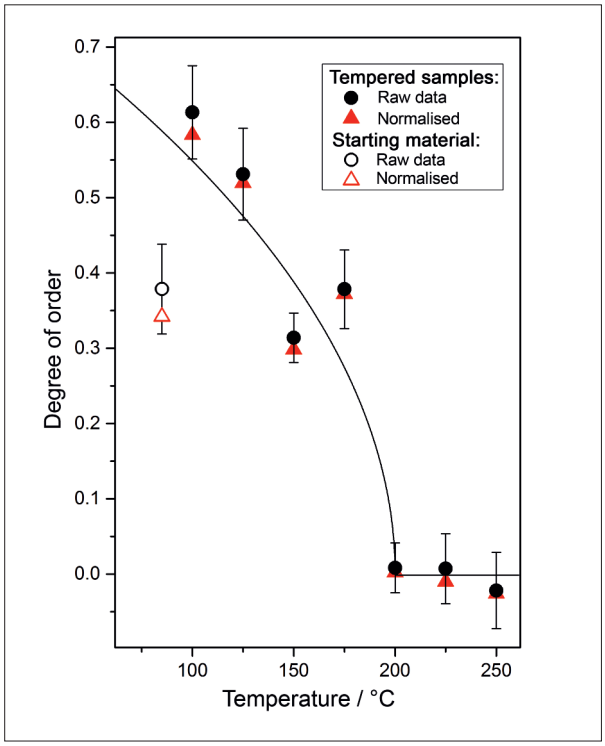
for use in photovoltaics, which can be up to 400 degrees Celsius. “That is why the change in their properties went unnoticed for so long,” Többens relates. “The cooling phase was simply deemed unimportant and so nobody observed it.”

Anomalous X-ray diffraction was the key

The defects to which he and his colleagues attribute the property changes are sites in the crystalline structure where copper and zinc atoms have switched places. Susan Schorr had already discovered some years ago, using neutron diffraction, that copper-zinc disorder exists in kesterites at room temperature. It has also long been known that such defects strongly influence the characteristics of the material. “So-called defect levels develop in the band gap of the semiconductor,” Többens explains. “Charge carriers can become caught in these, and thus no longer be able to contribute to the electric current.”
In order to determine the exact distribution of copper and zinc atoms and to observe the transition at different temperatures, the researchers had to perform an experimental trick. The usual analytical methods, namely neutron diffraction and conventional X-ray diffraction, were out of the question. “For more meaningful neutron diffraction experiments, you need larger sample quantities than can be manufactured perfectly reproducibly,” explains Daniel Többens. “Conventional X-ray analysis, on the other hand, is unsuitable because it cannot distinguish between copper and zinc atoms in the crystal.” This is because these two chemical elements have a very similar number of electrons. The researchers therefore found the solution in anomalous X-ray diffraction, diffraction experiments that use X-ray light of an energy exactly matching the absorption edges of the two elements. At these characteristic energies, copper and zinc can namely be distinguished from each other very easily. The photon source BESSY II at HZB delivered the exact wavelengths required for this.

An archetypal structural phase transition

There was just one last step that was missing: the scientists had to develop an entirely new analytical method to be able to interpret the data from their anomalous X-ray diffraction experiments. And the effort paid off. The results they obtained directly revealed for the first time what happens during the mysterious change in the crystal’s properties: the distribution of copper and zinc in the crystal structure transitions from a completely disordered state to an ordered state as it cools to below 203 degrees Celsius – a prime example of a structural phase transition. Because this happens at such low temperatures, highly ordered crystals with few defects can only be produced by very slow cooling.
“This insight has great significance for the further development of these materials,” says Többens. “We now have to find out how we can avoid the copper-zinc disorder, for example by a target-oriented substitution with other elements,” the department head Susan Schorr muses. “That way, we could optimise kesterites for photovoltaic applications.” *rb*



The degree of order of the kesterite studied decreases as temperature increases. At around 200 degrees Celsius, its degree of order is 0. This signifies complete disorder – copper and zinc are distributed randomly in the Cu-Zn layer. Complete order would be a degree of order of 1.

Phys. Status Solidi B 253, No. 10, 1890–1897, 2016 (DOI: 10.1002/pssb.201600372): Temperature dependency of Cu/Zn ordering in CZTSe kesterites determined by anomalous diffraction; D. M. Többens, G. Gurieva, S. Levcenko, T. Unold, and S. Schorr

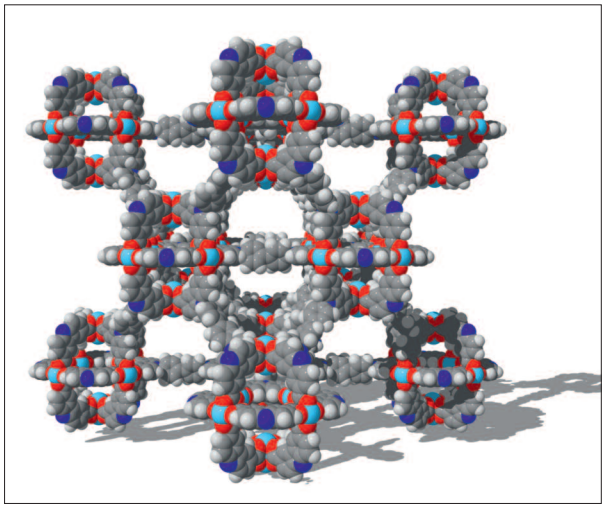
IN BRIEF

- Certain raw materials used in solar cells are already rare, for example indium, gallium, cadmium, arsenic and selenium. A team led by Prof. Dr. Susan Schorr is therefore researching kesterites as alternative absorber materials.
- Kesterites often exhibit defects in their crystalline structures at high temperatures. These defects drastically alter the electrical and optical properties of the kesterites.
- A team has managed to observe how these defects evolve in the crystals. Their next step is to control these processes in a targeted manner in order to optimise kesterites for photovoltaic applications.

ENERGY STORAGE MATERIALS UNDER PRESSURE

Metal-organic frameworks (MOFs) can store gases such as methane in their surface interstices, or pores. Teams from the Technische Universität Dresden and HZB have now precisely observed the process at BESSY II for the first time. They discovered a surprising effect: for MOFs reaching a specific pressure level, the gas **adsorbed eruptively escapes**. This suggests many new applications.

Methane is considered an ecologically friendly alternative to petrol and diesel fuel, especially if it is able to be produced from solar energy in the future. To fill automobile tanks with methane, suitable materials must be developed that can retain the gas without leakage. Being able to adsorb and store gases in their pores means metal-organic frameworks (known as MOFs) are candidates for this purpose. A team from Technische Universität Dresden has now developed an MOF by the name of DUT-49. The structure of DUT-49 contains relatively large spaces



The three-dimensional structural network of the ultra-porous and flexible material called DUT-49 can store large amounts of methane.

with diameters of 1.0 to 2.4 nanometres and can therefore adsorb extremely large amounts of methane – more than 300 grammes of methane per kilogramme of DUT-49 at room temperature. As a result, DUT-49 is being considered for methane storage in automobiles operated with natural gas or biogas.
In order to improve this material, the TU Dresden team headed by Professor Dr. Stefan Kaskel has now analysed the pressure and temperature dependence of gas adsorption and release together with the associated structural changes. Working together with experts headed by Dr. Dirk Wallacher and Dr. Daniel Többens at HZB, they developed a sample environment that enables the temperature and gas pressure to be adjusted during X-ray studies at BESSY II as well as being able to determine the quantity of gas that has been adsorbed.
The scientists were able to shed light on the crystal structure of the material using X-ray diffraction and X-ray absorption spectroscopy (EXAFS) at the BESSY II KMC-2 beamline, showing where the gas molecules are embedded in the pores of the crystal and how the framework deforms as a result. The sample environment utilised here, which made possible the controlled loading of the samples with various gases during measurements (in situ), was specially developed for the KMC-2 beamline under a project funded by the German Federal Ministry of Education and Research (BMBF). This project is a joint effort between TU Dresden, the HZB Sample Environment group, and the HZB Structure and Dynamics of Energy Materials department.

Eruption of gas from the contracting pores

During the experiments it was discovered that DUT-49 behaves more unusually than expected. When the pressure of the externally fed methane or butane gas is gradually increased, more and more gas molecules are initially adsorbed into the crystal and fill the tiny pores. However, if the gas pressure exceeds a threshold of 10 kilopascals for methane or 30 kilopascals for butane, the material's structural form closes off. The organic molecules that have stretched the framework become twisted and kinked, causing the pores of the structure to contract. The gas is then eruptively expelled from the material, and the crystal structure shrinks to less than half its volume. The volume of the pores is reduced even more, by about 61 per cent. The structure only gradually re-opens at still higher pressure, with pores of all sizes again filling completely with gas molecules. If the pressure is reduced once again, then the opposite process occurs and the open-pored structure is restored. However, this occurs only at very low pressures, an effect referred to as hysteresis.

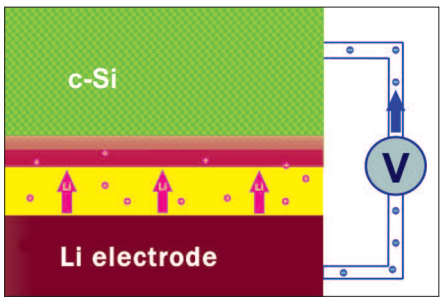
Quantum mechanical calculations by two French teams in Paris and Montpellier show that the different shape of the small pores in the closed form is especially favourable for deposition of methane molecules. At very high gas pressure, it is energetically more favourable if more methane is deposited into the large pores. At lower pressures, there is not enough methane present to close the pores.
Above a pressure threshold, the pores contract so quickly that the gas already adsorbed into the MOF is explosively expelled, raising the gas pressure even higher. After the pores have closed, the structure contains less gas then before, although the gas pressure is higher. This kind of "negative gas adsorption" is quite rare; the behaviour has never been observed in metal-organic frameworks before. It suggests new potential applications such as for the design of micro-pneumatic components in rescue systems, microengineering, and separation processes that react sensitively to changes in environmental pressure. *arö*

Nature 532, 348–352 (DOI: 10.1038/nature17430): A pressure-amplifying framework material with negative gas adsorption transitions; S. Krause et. al.

STORING ENERGY WITH SILICON THIN FILMS

The capacity of lithium-ion batteries might be increased theoretically by six times by using anodes made of silicon instead of graphite. A team from the HZB Institute of Soft Matter and Functional Materials has observed for the first time in detail how **lithium ions migrate into thin films of silicon**. It was shown that extremely thin layers of silicon would be sufficient to maximise the load of lithium.

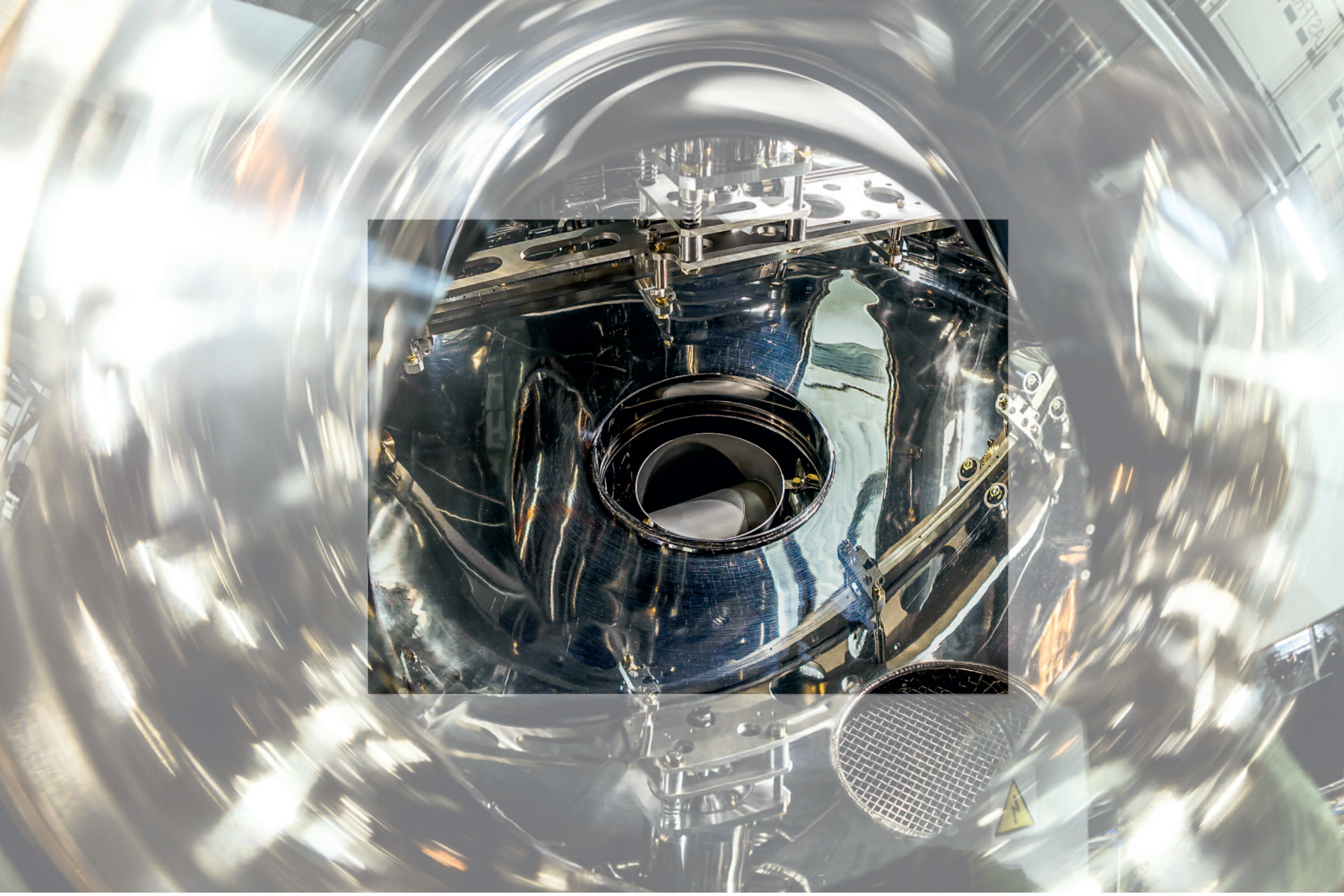
Lithium-ion batteries provide laptops, smart phones, and tablet computers with reliable energy. However, electric vehicles have not come as far along with conventional lithium-ion batteries. This is due to the currently utilised electrode materials such as graphite only being able to stably adsorb a limited number of lithium ions, restricting the capacity of these batteries. Semiconductor materials such as silicon are therefore receiving attention as alternative electrodes for lithium batteries. Bulk silicon is able to absorb enormous quantities of lithium. However, the migration of the lithium ions destroys the crystal structure of silicon. This can swell the volume by a factor of three, which leads to major mechanical stresses.
A team from the HZB Institute for Soft Matter and Functional Materials headed by Prof. Matthias Ballauff has now directly observed for the first time a lithium-silicon half-cell during its charging and discharge cycles. "We were able to precisely track where the lithium ions adsorb in the silicon electrode using neutron reflectometry methods, and also how fast they were moving", comments Dr. Beatrix-Kamelia Seidlhofer, who carried out the experiments. She discovered two different zones during her investigations. Near the boundary to the electrolytes, a roughly 20-nanometre layer formed that had an extremely high lithium content: 25 lithium atoms were lodged among 10 silicon atoms. A second adjacent layer contained only one lithium atom for ten silicon atoms. Both layers together are less than 100 nanometres thick after the second charging cycle.



Lithium ions migrate through the electrolyte (yellow) into the layer of crystalline silicon (c-Si). During the charging cycle, a 20-nanometre layer (red) develops on the silicon electrode, adsorbing extreme quantities of lithium atoms.

After discharge, about one lithium ion per silicon node in the electrode remained in the silicon boundary layer exposed to the electrolytes. Seidlhofer calculates from this that the theoretical maximum capacity of these silicon-lithium batteries lies at about 2300 milliampere-hours/gram. This is more than six times the capacity of a lithium-ion battery constructed with graphite (372 mAh/g). Therefore very thin silicon films should be sufficient for adsorbing the maximum possible amount of lithium, which in turn would save on the material and energy consumed during manufacture! *arö*

ACS Nano, 2016, 10 (8), pp 7458–7466 (DOI: 10.1021/acsnano.6b02032): Lithiation of Crystalline Silicon as Analyzed by Operando Neutron Reflectivity; B.-K. Seidlhofer et. al.



DEVELOPING METHODS FOR RESEARCH WITH SOFT X-RAYS

Facts & Figures from HZB

The nanocluster trap at BESSY II: nanoparticles comprising only a few to several hundred atoms are the link between individual atoms and expansive solid bodies. They can sometimes have radically different properties from the matter we know from our mundane macroscopic world. The intense X-ray light from the photon source BESSY II at HZB lets scientists research the magnetism of nanoparticles in extreme detail – but first they have to set the miniscule particles up in the right position.

In a joint project of the German Federal Ministry of Education and Research (BMBF), researchers from the University of Freiburg in close cooperation with HZB therefore developed a special ion trap for the tiny particles. The so-called Nanocluster Trap, installed in a permanent measuring station at BESSY II, keeps nanoparticles ensnared so that they can be cooled, magnetised and examined with X-ray light. The measuring station is now open to all scientists from around the world.

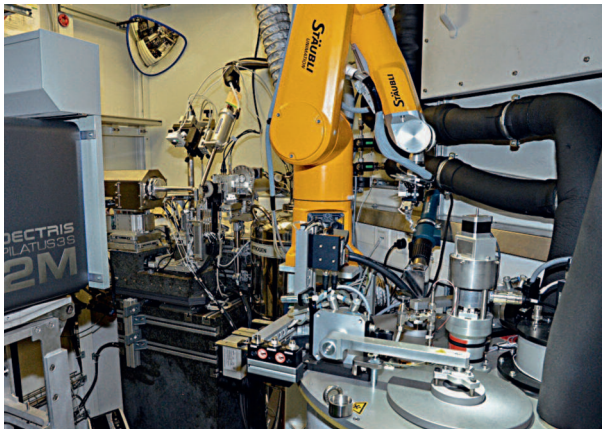
SPEEDING UP THE SEARCH FOR NEW DRUG MOLECULES

The macromolecular crystallography (MX) beamlines at the BESSY II X-ray source are specially designed for **highly automated structural analyses of protein crystals**. Teams from HZB and Philipps-Universität Marburg in Germany have successfully automated and demonstrated the evaluation of data records.

The search for new substances that are effective against a disease is like the first step in cracking a high-security lock: the active substance needs to fit into the target molecule like a key in a lock. The target molecule in this case is a protein, responsible for a specific function in an organism. The degree to which this function is accomplished can be influenced by active agents. Thus, an appropriate active agent can correct a function that has gone out of control and is causing a disease. However, first you need to identify an appropriate agent. And this search can be very tedious. Figuratively speaking, an infinite number of keys can be imagined, and it would take an infinite amount of time to test them all. An efficient safe-cracker will not spend forever checking an endless chain of keys, instead he will study the pins of the lock, one by one, until he can set each pin correctly. A similar procedure, called fragment screening, has become the conventional approach in structural biology. To discover a prototypal "blueprint", you assemble several individual fragments into a larger entity. To do so, you test hundreds of very small molecules (fragments) as to whether they bind to the target protein. A first lead structure for an active agent is then assembled from those fragments that bind.

A highly automated version of this procedure has already been running at the BESSY II MX beamlines for three years, facilitating a high throughput of samples. With over 2000 protein structures solved so far, the macromolecular crystallography beamlines at BESSY are by far the most productive ones in Germany. They are heavily overbooked, with demands originating from both academic and industrial research user groups.

Now a collaborative research project between the Philipps-Universität Marburg and HZB has succeeded in bringing this automation a step further. "We are able to work through hundreds of samples using fragment screening where manual evaluation is hardly feasible any more," says Dr. Manfred Weiss, who heads the HZB MX team. In collaboration with Prof. Gerhard Klebe and his group at Marburg, the teams jointly developed a computer program. It evaluates the raw X-ray crystallography data using an iterative process pipeline of evaluation routines and identifies those fragments that bind to the protein. Klebe's group has made the protein crystals available together with a library of different fragment molecules suitable for protein binding.



Each of the three MX beamlines at the photon source BESSY II offers specific characteristics for investigating protein crystals. Pictured here are MX beamlines 14.1 (top) and 14.2 (bottom).

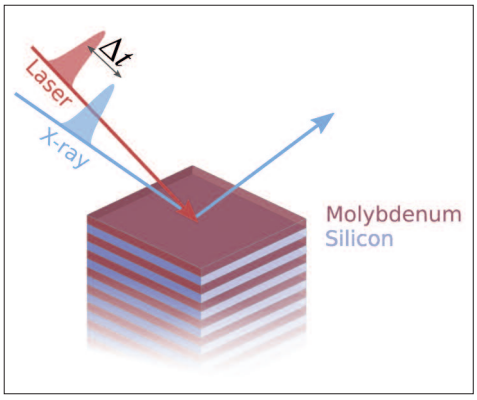
In collaboration, the partners tested the newly developed expert system using crystals of a specific protein soaked in total with 364 fragments in aqueous solutions. The expert system is also capable of automatically refining the X-ray structures. "Without this automated refinement procedure of the iterative expert system, a fair portion of the fragments would have remained undetected," Weiss explains. "For example, we had only identified about 50 candidates during the first evaluation while by using the iterative adaptive procedure, an additional 32 candidates could be discovered." The work shows that the new expert system allows more reliable detection of fragments that can be considered as suitable starting points or promising molecular portions for the development of potent active agents. This can speed up the search for new drug molecules. *arö*

Structure, Vol. 24, Issue 8, pp 1398–1409 (DOI: 10.1016/j.str. 2016. 06.010): High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits; J. Schiebel et. al.

VERSATILE CROSS-CORRELATOR FOR ULTRAFAST X-RAY EXPERIMENTS

In time-resolved, ultra-fast excitation query experiments, scientists must determine the temporal overlap between two emitted light pulses in order to obtain conclusive results. A team from HZB and the University of Potsdam has now found a new and surprisingly simple solution for precisely measuring this overlap even in experiments with **light pulses of different wavelengths**.

Electronic, magnetic and structural processes in energy materials take place on a timescale somewhere between several femtoseconds and a hundred picoseconds. In order to observe such processes, the sample is first excited by a "pump" light pulse and then probed by a time-delayed "probe" pulse. In any of these time-resolved pump-probe experiments, the vital prerequisite is to know the exact spatial and temporal overlap of the pump and probe pulses on the sample of interest. The problem of the temporal overlap had been previously solved by the laser community for two optical light pulses by using non-linear crystals to achieve temporal overlap. Unfortunately, no materials were found for correlating optical and X-ray pulses in a similar manner.



The X-ray reflectivity of the Mo/Si multilayer mirror is altered by a time-delayed laser pulse.

The main goal for the team from HZB and the University of Potsdam was to find a versatile method for cross-correlating a broad range of X-ray and laser photon energies on the different timescales from 100 femtoseconds to 100 picoseconds, as are available at BESSY II. They chose a standard molybdenum-silicon (Mo/Si) multilayer mirror as optimised for the soft X-ray regime. Such mirrors consist of alternating metallic molybdenum and semiconducting silicon layers of nanometre thickness, which result in so-called superlattice Bragg peaks that reflect X-rays from approximately 100 eV up to the hard X-ray regime with an efficiency of up to 70 per cent.

Using a laser with 50-femtosecond-long pulses of 800 nanometre wavelength, the experimentalists optically excite the Mo/Si mirror which leads to absorption of light only in the metallic molybdenum layers. This ultrafast heating of only every second layer results in the quasi-instantaneous excitation of coherent acoustic phonons that strongly modulate the reflectivity of the Mo/Si mirror on two different timescales. First, a fast intensity oscillation of the superlattice Bragg peaks of up to 10 per cent amplitude and 600 fs oscillation period and, second, a strong shift of the superlattice Bragg peak on a 10-picosecond timescale with more than 20 per cent transient signal change up to nanosecond delays. As initially desired, both effects allow for easily finding the temporal overlap of X-ray probe and laser pump pulses over a broad range of timescales.

Easy implementation and successful use

The presented technique is not only applicable for a broad range of photon energies but also requires no changes to the available sample environment, since the excited dynamics is independent of external fields and temperature, and can even be probed under ambient conditions. Additionally, the Mo/Si mirror used is extremely resistant against laser X-ray and/or oxidation damage. The possibility to change the mirror parameters combined with the deep understanding of the underlying ultrafast structural dynamics in such multilayer mirrors allows further optimisation and adaptation of this concept for special applications.

Recently, the Mo/Si cross-correlator was successfully used at UE52/SGM within the transmission NEXAFS chamber to precisely determine the temporal overlap of BESSY II's hybrid bunch and laser pulses from the newly built MHz system. *arö*

Struc. Dyn. 3, 054304, 2016 (DOI: 10.1063/1.4964296): Versatile soft X-ray-optical cross-correlator for ultrafast applications; D. Schick et. al.

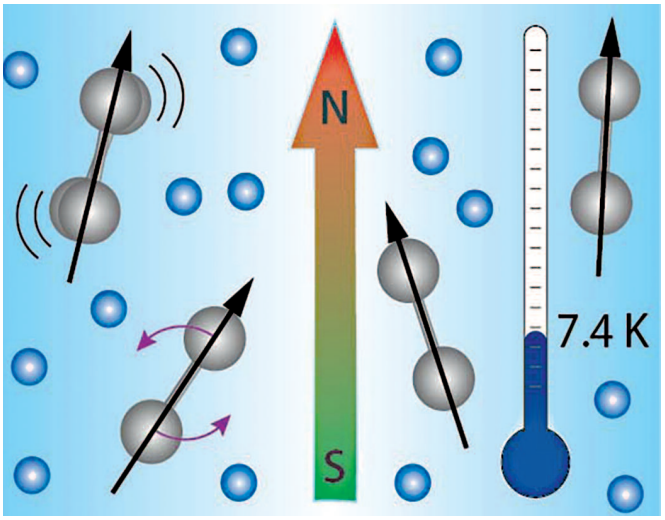
A NEW RECORD FOR SETTING AN ION TRAP

An international team has set a new temperature record for what are known as quadrupole ion traps that capture electrically charged molecular ions. The ion trap with this new method provides a new opportunity to study the magnetism and ground states of molecular ions and thus to develop new materials for **energy-efficient information technologies**.

The scientists from Sweden, Japan, and Germany succeeded in cooling about ten million ions down to 7.4 kelvin (approx. -265.8 degrees Celsius) using a buffer gas. That is a new record. Previously it was only possible to cool down about one thousand ions to 7.5 K using a buffer gas. However, a thousand ions are not nearly enough for spectroscopic analyses. “Until now, everyone assumed it would not be possible to reach lower temperatures at such a high density of ions with a quadrupole ion trap. But it can be done”, says HZB researcher Dr. Tobias Lau. This is because the RF electromagnetic field doesn't just trap the stored ions, but “jiggles” them as well so they are constantly gaining energy and rising in temperature. In order to draw off this additional energy, the team introduced helium as a buffer gas, and at a relatively high pressure. “You have to imagine this as kind of a cold syrup that damps the macro motion of the particles, slowing their rotation and translation”, explains Dr. Vicente Zamudio-Bayer from the University of Freiburg.

Magnetic moments of N2 cations

The experiments were carried out using the UE52-PGM station at BESSY II where polarisation of the soft X-ray radiation can be varied. The experimental set-up at this beamline is unique in facilitating X-ray spectroscopy of cryogenic ions under externally applied magnetic fields. The sample can be analysed in an externally applied magnetic field using circularly polarised X-rays (X-ray magnetic circular dichroism/XMCD). This yields information about the magnetic moments of the electrons subdivided into both spin and orbital contributions.
“We were able for the first time to experimentally determine the magnetic moments of nickel dimer cations thanks to the especially low temperatures”, Lau continued. The work on the ion trap is part of a larger project of HZB and the University of Freiburg being funded by the German Federal Ministry of Education and Research (BMBF). “We are now working on reaching even lower temperatures.



Diatomic nickel ions (grey) are captured at cryogenic temperatures in an RF ion trap; cold helium gas (blue) serves to dissipate the heat. The magnetic field orients the ions.

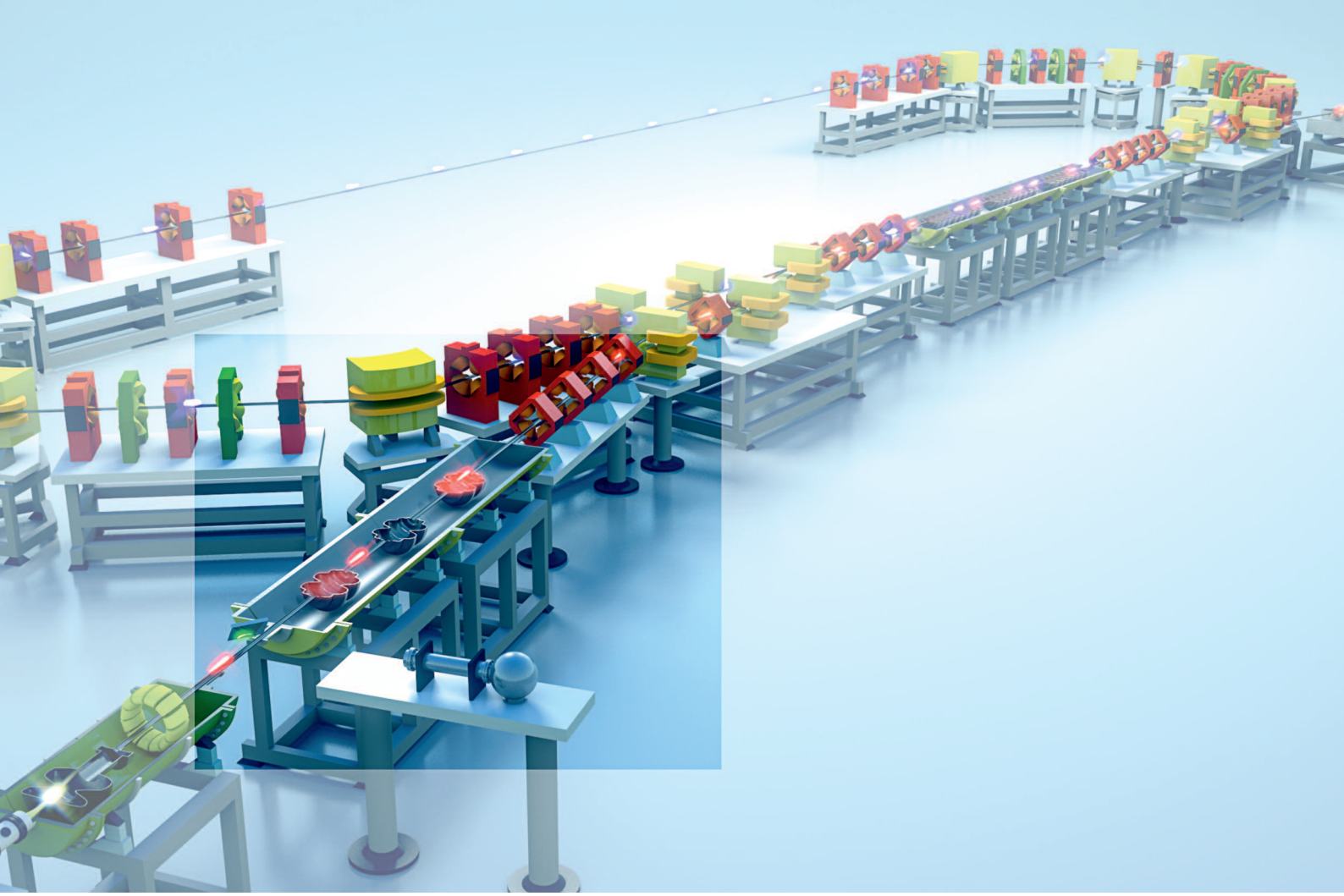
We hope we will soon get to 5 K”, offers Zamudio-Bayer. The lower the temperature, the more clearly the magnetic effects show up.

User can benefit from the ion trap already

All users of the ion trap at the BESSY II UE52-PGM station can benefit already from the record achieved. “Not only magnetism, but also many other properties of a wide range of different molecules can be studied spectroscopically here, such as transition-metal ion complexes. That will therefore be attractive to many users, especially those in physical chemistry”, Lau thinks.

arö

Journal of Chemical Physics 145, 194302, 2016 (DOI: 10.1063/1.4967821): Electronic ground state of Ni_{2+}, V. Zamudio-Bayer, R. Lindblad, C. Bülow, G. Leistner, A. Terasaki, B. v. Issendorff, and J. T. Lau



ACCELERATOR RESEARCH AND DEVELOPMENT

Facts & Figures from HZB

HZB is setting up a new application laboratory: HZB is receiving 7.4 million euros from the European Regional Development Fund (EFRE). The money is being used to set up the application laboratory "SupraLab@HZB" for the advancement of high-current superconducting cavities. These components will be needed for operating the next generation of novel, high-performance light sources. The laboratory will also provide complex superconducting component test beds for use by companies and research institutes in the region.

To set up the new application laboratory, HZB is applying its internationally renowned expertise in the development of continuous wave (CW) superconducting accelerator components. "The advantage of these CW superconducting cavities is that they permanently apply a very high accelerator field and at the same time provide the freedom to optimise the geometry for high-current mode," says Prof. Dr. Jens Knobloch, head of the HZB institute "SRF – Science and Technology" (ISRF), which has assumed the scientific direction of the SupraLab: "So not only do they accelerate a high electron current; they also offer a practically freely selectable time structure – the pulse sequence – of the current. Thanks to the EFRE funding, we now have the opportunity to develop this technology a great deal further until it is ready for application in light sources."

The project is being funded as of 1 January 2017, and will run until the end of 2019. Helmholtz-Zentrum Berlin is contributing an equal sum from its own means.

HZB ON ITS WAY TO THE LINEAR ACCELERATOR

The shell for the bERLinPro building – the test facility for an **energy-recovery linear accelerator** at Helmholtz-Zentrum Berlin – is now complete. The extremely complex structure was erected at the Wilhelm Conrad Röntgen Campus of HZB in Berlin-Adlershof in just ten months – the topping-out ceremony took place in July 2016.

Prof. Dr. Andreas Jankowiak, head of the HZB Institute for Accelerator Physics and the bERLinPro project is confident: "bERLinPro will be a unique research instrument with which we will enter completely new territory in accelerator technology". This involves the prototype of an energy-recovery linear accelerator in which electrons will be accelerated with large amounts of energy to almost the speed of light. Electrons in this state emit high-quality X-rays that are very important for research purposes. After passing through the high-speed sections of bERLinPro, the electrons will be captured again and their remaining energy recovered. "To realise bERLinPro, we first need to develop the various components and methods, and then test them in the new accelerator hall", explains Prof. Jens Knobloch, head of the SRF - Science and Technology Institute that has a major role in the development of bERLinPro. "A rather complex infrastructure is necessary for this." The construction of the hall has therefore been a demanding project. "The planners needed to take into account the demands for increased radiation protection and statics, for example. For this reason, just the erection of the structural shell represented an enormous challenge for the companies participating in the construction and their staff. Not least of which was realisation of the operational infrastructure, such as guaranteeing proper operation of the cooling system for the superconducting test accelerator that will be tackled next", elaborated Dr. Birgit Schröder-Smeibidl, until the autumn of 2016 head of the HZB Facility Management division, and under whose supervision the hall has been constructed. Constanze Tibes, the architect for the building (DGI-Bauwerk architectural GmbH), added: "There was no other building we could take as an example for the hall and planning was very time-consuming. We have erected here a unique structure for serving science."
"Completing this work in such a short time was only feasible because all those involved have worked together in an outstanding manner", emphasised the engineer responsible for the project at HZB, Oliver Schüler. "Communications were superb and enabled us to adhere to all the scheduling and cost projections."

The topping-out ceremony took place on July 27, 2016, in the presence of construction firms, guest VIPs, and HZB staff.

Utilising both long- and short-duration packets of electrons simultaneously with BESSY-VSR

A number of the components that have been developed for bERLinPro can be incorporated for use in the BESSY II electron storage ring. This is the case, for example of the high-current superconducting cavity resonators that accelerate the electrons. They constitute the centrepiece of BESSY-VSR, the variable pulse-length storage ring that BESSY II will be converted into next.
While packets of electrons of only a particular duration circulate in BESSY II, researchers want to simultaneously utilise both long- and short-duration packets of electrons in BESSY-VSR to create long and short pulses of light within the same ring. "The synergies between the two projects will begin to benefit the future users of BESSY-VSR during the period when we are still preparing components in the test facility for employment in bERLinPro", confirms Prof. Anke Kaysser-Pyzalla, Scientific Director of HZB: "Researchers, in particular those who depend on short pulses, are enthusiastic about our design for BESSY-VSR and the advantages that bERLinPro development will introduce."

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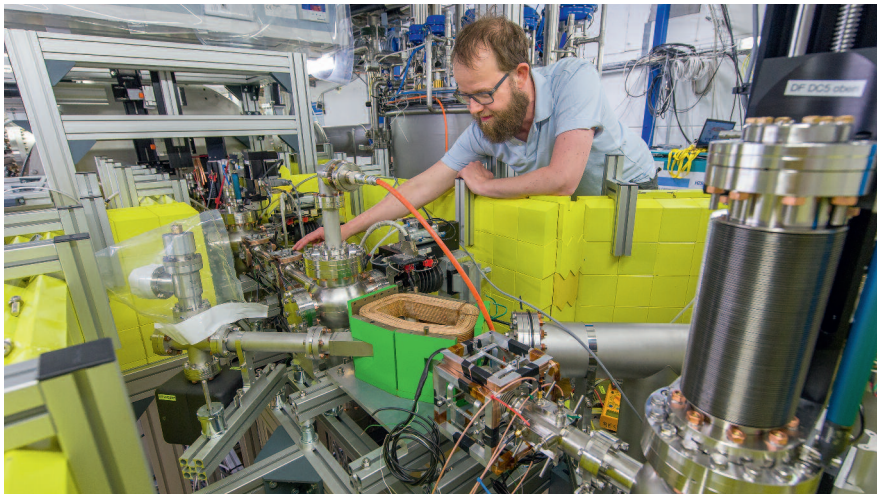
THE ELECTRON SOURCE IS TAKING SHAPE

Since autumn 2015, HZB has been steadily working on its future project bERLinPro in Adlershof – building a compact test facility for an **energy recovery linac (ERL)**. The project team has come one step closer to realising this technologically unique project with completion of the electron beam generation facility.



Dr. Thorsten Kamps of the HZB Institute for Accelerator Physics is part of the team developing the system that generates the electron beam for bERLinPro in the GunLab.

This is the stage where the team members of the future project bERLinPro would normally pause to admire the culmination of their efforts, but there's barely enough room to stand, let alone to take a good picture. The prototype of the facility that will one day produce the electron beam for the future energy recovery linac bERLinPro is located in a room called the GunLab, which is about 75 square metres large and jam-packed with high-tech equipment. There is just enough room against the walls for two people to squeeze past each other if they both hold in their stomachs. But taking pictures is hardly a concern for the physicists Dr. Thorsten Kamps, Dr. Guido Klemz, Dr. Julius Kühn, Dr. Axel Neumann and some twenty more team members. Their interest lies in accelerating the extremely bright electron packets, or "bunches", destined for feeding into future accelerator facilities – such as the prototype of the energy recovery linac bERLinPro, currently being built at HZB.

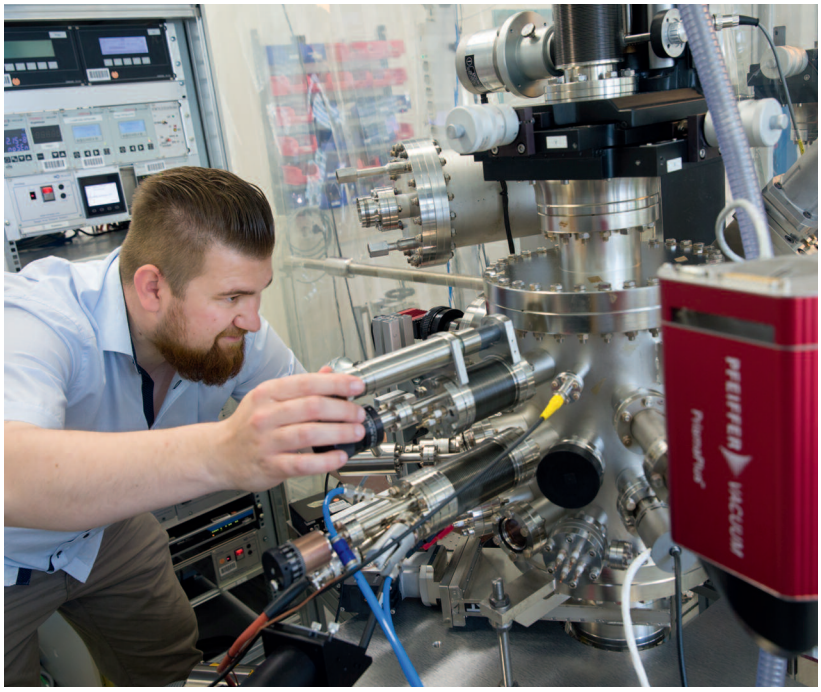
Last year, the scientists and engineers made great strides forward in this project. Four essential components for producing the electron bunches were developed and built to testing maturity: a potassium-caesium antimonide semiconductor photocathode that releases the electrons; a laser that fires light pulses of different wavelengths and durations at this cathode; a superconducting high-frequency cavity in the cooling system, called a cryomodule, in which electromagnetic fields accelerate the bunches to near light speed over very short distances, and a beam diagnostics beamline for precisely measuring the important beam parameters of length, shape and emittance (the product of divergence and beam area). The photocathode, laser, high-frequency cavity and beam guide can now be combined together and tested as an ensemble in the GunLab. By the beginning of 2018, the electron beam generation capability should be at the stage where it is ready for bERLinPro.

Reproducible cathodes of high quantum efficiency

In charge of the photocathode is Julius Kühn. Together with his colleagues, he investigated the best conditions for reacting potassium and caesium with antimony in order to produce a semiconductor cathode of highest quantum efficiency: "In the cathode laboratory, we vapour-deposited the ingredients in various proportions and orders onto highly pure, polished molybdenum plugs, and then tested the performance of the cathode immediately where it stood," Kühn explains. "We are working on an optimised manufacturing method that can make the cathodes reproducibly and with high quantum efficiency. High quantum efficiency means that each photon knocks as many electrons out of the surface as possible."

A high-power laser delivers the photons in the form of ultra-short light pulses, as Guido Klemz explains. Klemz is in charge of laser technology in photo injectors and

accelerators: “We boosted an existing laser to the point where it can now produce light pulses of variable durations from 10 to 20 picoseconds and at different wavelengths.” This variability of the wavelengths, and with it the energy of the photons, is important because the researchers are starting by generating the electron beam with a simple copper photocathode first before moving on to the more vacuum-sensitive technology of semiconductor photocathodes.
This copper cathode is highly stable and has ample quantum efficiency when irradiated with ultraviolet light. The semiconductor photocathode to be used later, consisting of potassium-caesium antimonide, has high quantum efficiency in the green range of the light spectrum. “We can produce these different wavelengths using special lenses in which the light passes through optically nonlinear crystals,” says Guido Klemz.
To develop their high-power laser, the HZB scientists cooperated intensively with the Max Born Institute, “and we will continue this cooperation into the development of the laser system that will be needed later for bERLinPro,” says Prof. Dr. Andreas Jankowiak, head of the HZB Institute for Accelerator Physics and project manager for bERLinPro. “Collaboration with our MBI colleagues is very important for this.”



Dr. Julius Kühn in the photocathode lab where the semiconductor cathode was researched.

A pristine resonator

The lasers and photocathodes were thus technologically ready to be combined with the third key component in the GunLab: the superconducting high-frequency resonator, in which alternating electromagnetic fields accelerate the electron bunches to near light speed. Prof. Dr. Jens Knobloch is head of the HZB institute SRF – Science and Technology and in charge of resonator development. “The resonator, created in collaboration with the US Jefferson Lab, is extremely sensitive to contamination by even the tiniest of foreign particles, such as microscopic dust particles only a few thousandths of a millimetre in diameter.” Accordingly, all integration and attachment of cooling units, high-frequency transmitters and other components had to be done in a clean room under the most particle-free conditions possible.
As tests of the high-frequency characteristics showed, the team did so with success. “The resonator builds up very high, stable fields,” says Axel Neumann, one of the physicists in Knobloch’s team who was heavily involved in the development and installation of the resonator. “It attains the planned values precisely; deviations are within the range of measurement accuracy. Next, we will actually be able to install the photocathode and fire laser light pulses at it.”
Again, this will demand utmost precision and attentiveness at all times to ensure the resonator is not contaminated in any way. The success of this endeavour will be seen when the full facility is tested in the second half of 2017. “By the end of January 2018, we must be finished with all tests,” says Thorsten Kamps from the Institute for Accelerator Physics. “If all goes well, we will have then shown how we can build a worldwide unique electron source to feed bERLinPro with electron bunches of superlative quality.” Finally, the ultimate task is to accelerate the electrons to high energy and then recover this energy once they have passed through the entire system. Thus, there will be no shortage of challenges in future. *hs*

IN BRIEF

- On its Wilhelm Conrad Röntgen Campus in Berlin-Adlershof, HZB is developing a prototype of the energy recovery linac bERLinPro.
- Scientists and engineers have developed and built four essential components for producing the electron bunches, which are now ready for testing.
- By the end of January 2018, they will have performed extensive testing to show how a worldwide unique electron source can be built to feed bERLinPro with electron bunches of superlative quality.

In hot demand: the 11,992.5 eight-hour experiment shifts available on 26 instruments at the synchrotron source BESSY II were used to 100 percent in 2016.

Planning for the long term: Helmholtz-Zentrum Berlin is one of seven Helmholtz centres working on system solutions for our future energy supply with renewable energies.

FACTS AND FIGURES ABOUT HZB

26
percent of radiation time at BESSY II in 2016 was for HZB internal use.

76
cooperative partnerships between HZB and companies were newly established in 2016 alone. Thus the total number of ongoing cooperative partnerships with industry more than doubled from 53 in the previous year to 109. Of these, nearly 46 per cent were cooperatives with companies from outside Germany and nearly 30 per cent cooperatives with small to mid-sized businesses.

7,504
hours (938 shifts, 312.27 days) were dedicated to scientific use of the storage ring facility BESSY II in 2016. This equates to 69 per cent availability. 1,168 hours (146 shifts, 48.67 days) were reserved for accelerator experiments.

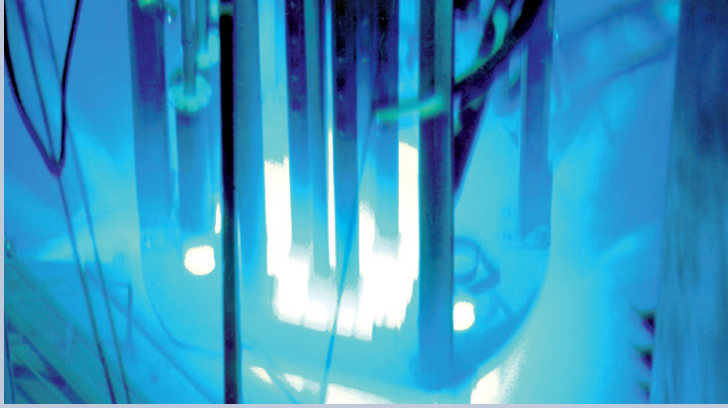
137
cooperatives were maintained by HZB with other scientific establishments at the end of 2016.

45
adolescents and young adults were receiving training at HZB at the end of 2016, 14 of whom were aiming for their Bachelor of Science (BA) in computer engineering (12) and mechanical engineering (2). HZB was also training 31 young people in seven professions, including six “system integration” IT engineers, four precision engineers, four mechatronics engineers, and one electronics engineer for operating technology. In fiscal 2016, HZB closed a total of eleven new training contracts with trainees. In the scope of cooperative training with Helmholtz-Zentrum Potsdam, another four trainees were accepted for a one-year training segment at HZB as physics laboratory assistants.

22
per cent of the 664 scientific employees at HZB are women. The proportion of women among all 1,141 employees is 28.2 per cent.

10
patents were granted to HZB in 2016. At the end of the year, HZB’s portfolio amounted to 251 patents, 21 of which are objects of ongoing licence agreements. 9 invention disclosures from 2016 were evaluated by HZB or external technology experts with regard to their patentability and/or commercial exploitability.

Hugely popular: the two HZB School Labs offer project days for schools from primary to tertiary level and teacher training. Experimenting is a playful way to introduce children and adolescents to science.



Well utilised: 1,659.5 instrument days were available for regular user operation at the research reactor BER II in 2016. Operation of BER II will be discontinued at the end of 2019.

197

PhD students were supervised at HZB in 2016. The number of theses completed in the same year was 31.

6.786

million euros were received by HZB for technology transfer in 2016. A little more than one million euros came from research and development partnerships and from R&D orders with domestic and international commercial enterprises, and around 3.27 million euros from other R&D cooperatives. Another 2.18 million euros originated from infrastructure agreements.

457

ISI- or SCOPUS-cited publications were published by scientists at HZB in 2016.

175.5

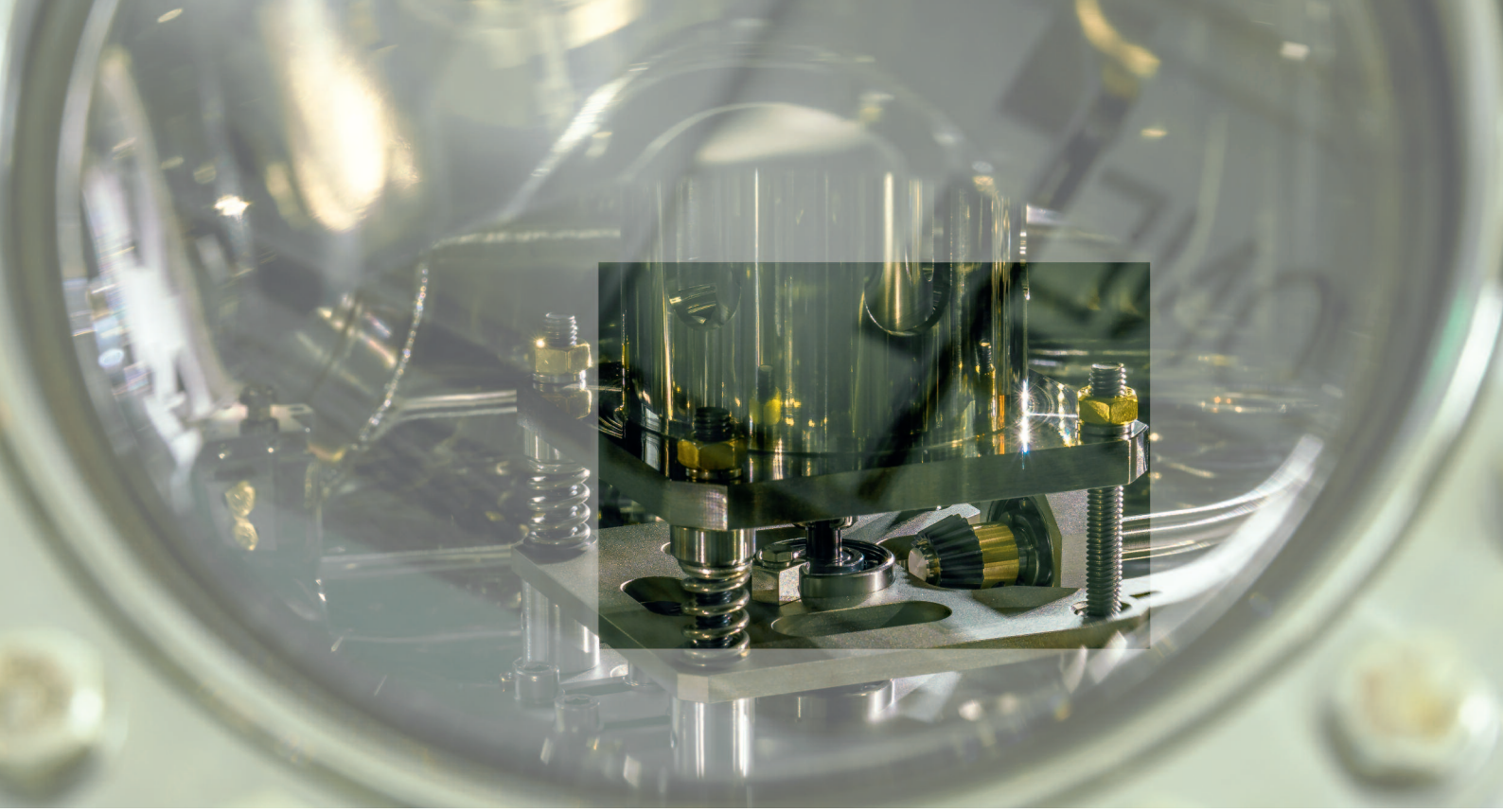
days over 11 reactor cycles were clocked for powered operation of the research reactor BER II in 2016. This equates to a total of 1,659.5 instrument days of regular operation on 13 instruments in the first half of the year and 9 instruments in the second half of the year. 272 instrument days were needed for instrument development and maintenance, another 49 for the final commissioning of HFM/EXED, and on one day the instruments were down for technical reasons. The remaining 1,337.5 experimental days were used for the experiments of internal and external guests.

22.8

million euros in third-party funding went to HZB in 2016. This included around 5.4 million euros for contract research, 3.66 million euros for services for third parties, around 2.9 million euros in project funding from the federal government, and nearly 2 million euros from the European Union.

2,800

school students attended the two School Labs in Wannsee and Adlershof in 2016. Four groups of pupils were from abroad, and four groups came in field trips and class excursions from other parts of Germany.



HIGHLIGHTS FROM USER EXPERIMENTS

At the 8th Joint BER II and BESSY II User Meeting held in December 2016, two scientists were awarded the Ernst-Eckhard-Koch Prize for outstanding doctoral theses in the field of research with synchrotron radiation. **Dr. Joachim Robert Gräfe** of the Max Planck Institute of Intelligent Systems in Stuttgart was recognised for his doctoral thesis "Static and dynamic magnetisation properties of nano-scale superlattices" at the University of Stuttgart. During his doctoral studies, he accomplished the world's first direct mapping and analysis of spin waves, also referred to as magnons, in nanoscale anti-dot lattices with the help of dynamic X-ray microscopy at GHz frequencies. He performed his experiments on the MAXYMUS microscope at BESSY II.

Dr. Jan Wernecke, who now works for IAV in Gifhorn, was recognised for his doctoral thesis "When size does matter: Dimensional metrology of nanostructured layers and surfaces using X-rays" at the Technische Universität Berlin. He carried out his studies in the BESSY II laboratory of the Physikalisch-Technische Bundesanstalt (PTB), Germany's national metrology institute. The main task was to measure nano-dimensional features on surfaces using small-angle X-ray scattering and to establish metrological traceability back to the international system of units, SI, with uncertainties in the range of a few atomic diameters.

Dr. Christian Tusche of Forschungszentrum Jülich was awarded the 2016 Innovation Prize Synchrotron Radiation at the Joint User Meeting. Thanks to his pioneering paper "Imaging spin filters for spin-resolving momentum microscopy", which substantially resulted from work done at the Max Planck Institute (MPI) of Microstructure Physics in Halle and at BESSY II, the efficiency of spin-resolved electron spectroscopy can be increased by up to four orders of magnitude.

X-RAY CORELAB NOW AVAILABLE FOR USE

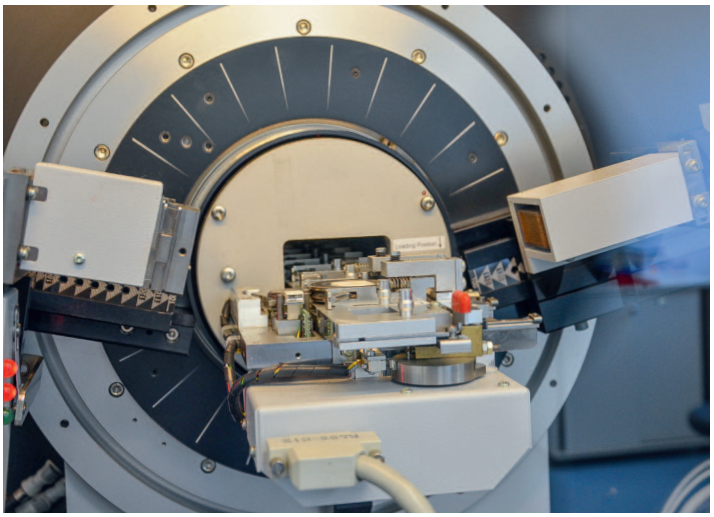
At the X-Ray CoreLab, HZB combines a diverse range of **X-ray diffractometry equipment** for scientists to use. Each instrument is specialised for specific experiments – and is state of the art.

X-ray diffractometry is one of the most important analytical methods in materials research. It is employed frequently at HZB for many different purposes, including developing new materials for energy conversion or storage. It is suitable for both thin-film analysis and classic crystal structure analysis of either powder samples or single crystals. While there are many instruments available at BESSY II for studying complex thin-film systems, not all experiments require the high-intensity, brilliant synchrotron radiation from the storage ring. HZB therefore provides instruments that operate with a classic X-ray source.

The most important devices have now been brought together to make them available to all scientists in the X-ray CoreLab. The idea was initiated by Prof. Dr. Christoph Genzel and developed by Prof. Dr. Susan Schorr, Head of the X-ray CoreLab Steering Committee. New laboratory space was set up for this over the last few months in the basement of the PT Building at the Lise Meitner Campus of HZB's Wannsee location. There are now five X-ray diffractometers available here for analysing thin films and powder samples, and two for investigating single crystals. "All the instruments were brought up to current technical standards during the move and equipped with the newest versions of hardware and latest software releases", says Michael Tovar who is in charge of laboratory operations. As a result, Wannsee now also has the capability of carrying out texture and epitaxy studies on thin films, which was previously a bottleneck at this location.

The X-ray CoreLab on the Wilhelm-Conrad-Roentgen-Campus in HZB's Adlershof location falls under the responsibility of Christoph Genzel and comprises three devices. There are two diffractometers in Laboratory R 6106, including a new 8-circle diffractometer. These instruments allow depth-resolved analysis of near-surface gradients such as residual stresses, texture and microstructure of polycrystalline materials and thin films.

Two high-flux MetalJet sources are among the highlights of the new X-ray CoreLab, one located in Berlin Wannsee (room LS012) and one in the EMIL Lab in Berlin-Adlershof. The Metaljet sources are still in the process of being set up and will be available to CoreLab users after successful commissioning.



The X-ray diffraction devices in the HZB X-ray CoreLab are available to all scientists.

Instrument time via the online calendar

The instruments at the X-ray CoreLab are available for all HZB staff and visiting scientists to use for their research. External scientists can also apply for instrument time and use the X-ray CoreLab as of 2017. "Numerous scientific questions can be answered with the help of our pool of devices in the X-ray CoreLab without necessarily resorting to large-scale facilities such as BESSY II, because instrument time there is more expensive and, especially, quite limited," says Susan Schorr. The lab's infrastructure excellently complements research conducted at the large-scale facilities and is a component of the new HZB strategy. If you wish to use an instrument, you must first become an X-ray CoreLab user. The X-ray CoreLab website, available at www.helmholtz-berlin.de/forschung, provides the instrument specifications and details of the people to contact. *red*

HOW WATER MOVES GLASS

Using an artificially **petrified conifer cone,** scientists at the Chair of Biogenic Polymers of the Technical University Munich, located at the Science Center Straubing, laid the foundations for a new generation of sensoric materials.

Plants use capillary forces to draw fluids upwards against gravity. Capillaries are very thin tubes, and the network of capillaries in plants causes the plant material to expand when they soak up fluids. This even happens inside the cones of conifers. The WZS researchers wanted to know whether this effect can be exploited for other uses. “For the first time, we applied a previously developed and refined ‘bio-templating’ process to create materials with structure-based functionality,” says Dr. Daniel Van Opdenbosch, who works at the Science Center Straubing. With the bio-templating process, one can artificially petrify pine cones: the biological components are completely transformed into the technical material silica glass.

A new generation of sensors: The scales of the petrified cone move upwards against gravity, and on drying back to their starting positions

Elaborate analyses at the µSpot Beamline at the synchrotron source BESSY II in Berlin showed that the internal structure of the pine cone was fully retained. The µSpot beamline and corresponding experimental station were operated in cooperation with the so-called “Cooperative Research Groups” of the BAM and the Max Planck Institute of Colloids and Interfaces in Potsdam-Golm. “The µSpot was designed so that many different methods can be applied to hierarchically structured samples such as wood, bone, catalysts, or archaeological finds. We used absorption spectroscopy to study the atomic properties, Raman spectroscopy for the molecular composition, diffraction for the crystalline structure, and small-angle scattering for the nanostructure,” explains Dr. Ivo Zizak, who is responsible for this beamline at HZB. “An online microscope delivers the macroscopic structure of the sample. The X-ray beam is focused to a few microns and, by 2-D or 3-D scanning, we can combine microscopic information with the macroscopic.” This combination of different methods into one experiment allows one to investigate the dependency between crystalline structure and atomic composition. The researchers used small-angle scattering to study the nanostructures of the cones, in particular the alignment of fibrils and pore sizes relative to their position in the cone scale.

Sensors can be created with little technical effort

In cooperation with the Institute of Physics of Montanuniversitaet Leoben, Austria, the new bio-templating process petrified the cone completely and accurately down to the smallest hierarchical level of only millionths of millimeters. Van Opdenbosch explains “we could induce the obtained samples to move in a similar manner to their biological originals during the uptake of moisture. The scales of the petrified cones move upwards against gravity, and then, on drying, back to their starting positions.“ The scientists hope the precise templating of plant structures and the corresponding retention of their characteristic properties will be a pathway for the development of functional materials. Based on the current results, they assert that porous ceramic multilayer sensors can be prepared at comparatively low expenditure. Such novel sensors react to changes in moisture with angular movement. They could therefore be used for measuring, switching or controlling in chemically or physically aggressive environments.

TU München/WZS

Advanced Materials, Vol. 28, Issue 26, pp 5235-5240 (DOI: 10.1002/adma.20160 0117): Moisture-Driven Ceramic Bilayer Actuators from a Biotemplating Approach; D. Van Opdenbosch et. al.

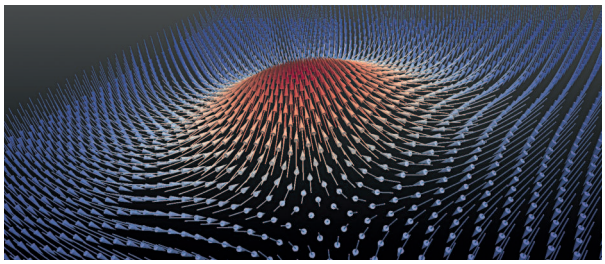
PING-PONG WITH SKYRMIONS

Bizarre vortices in magnetic fields – **called skyrmions** – could one day become a component of novel storage media. Two international research teams have established a basis for this through their work at HZB.

From its name alone, this bizarre solid-state physical phenomenon sounds like it could be straight out of science fiction. A skyrmion is a nanoscale magnetic structure that somehow resembles the whorl of hair at the back of one's head, and proves just as difficult to smooth down. Researchers first observed them experimentally in 2009, albeit only under extreme conditions, namely inside an exotic crystal at temperatures approaching absolute zero at around minus 273 degrees Celsius.
Under these conditions, there are no conceivable practical applications for this particle-like field vortex. Nevertheless, skyrmions are more than just a curious magnetic model system; they are genuine candidates for future compact, energy-saving data storage media. Their tiny dimensions, their relatively high stability compared to other structures, their low susceptibility to effects from local defects in the material, and yet their ability to be directly influenced by electrical current all represent great advantages.
The results of two international research teams at HZB have now brought the goal of using skyrmions for data processing much closer. Scientists led by Seonghoon Woo from the Massachusetts Institute of Technology (MIT) in Boston have shown, for example, that the magnetic vortex can also be produced in conventional ferromagnetic materials stacked on top of one another as several ultra-thin layers – not in extreme cold, but at ordinary room temperatures. Woo and his colleague researchers also succeeded in shifting vortex packets back and forth in a targeted manner between two positions. Positions and distances between skyrmions could represent digital states such as ones and zeroes, for example. Each skyrmion, the idea goes, would represent a single bit of data – a job currently fulfilled by much larger, or locally bound, packets in today's storage media.

Arbitrarily repeatable digital states

For the purpose of storing, reading and deleting data, one must be able to manipulate the vortex not only once, but as many times as desired. Results obtained from experiments performed by a team led by Kai Litzius from the Institute of Physics of the University of Mainz proved this to be possible.



The magnetic structure of a skyrmion is ordered symmetrically around its core, making it look identical from all sides. In this illustration, the arrows indicate the alignment of the spins.

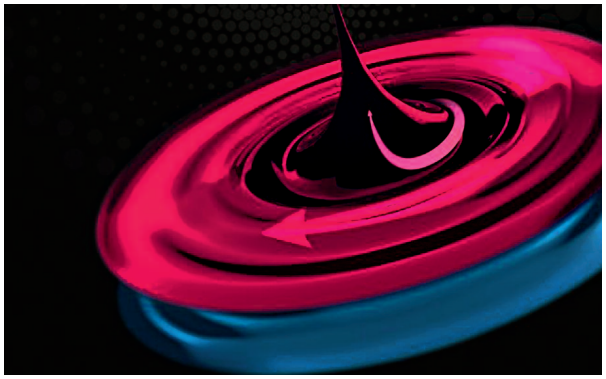
The researchers demonstrated it using the so-called Hall Effect, where a magnetic field applied perpendicularly to moving electric charges deflects them from their path. Vice versa, an electric current in certain materials, typically thin films of heavy metals, can also produce an accumulation of magnetic moments (spins), which then invoke a change in the spin structure of a second magnetic layer. Thus, skyrmions can be reproducibly pushed to and fro, as Litzius and his research colleagues showed. "This controlled deflection of the magnetic vortex was repeated more than a billion times, reliably and error-free," reports Dr. Markus Weigand. He heads the X-ray Microscopy workgroup in the Modern Magnetic Systems department of the Stuttgart Max Planck Institute for Intelligent Systems, which operates a high-resolution X-ray microscope at HZB. Both research teams used this facility for their skyrmion experiments.
Weigand sees the results as "a giant leap forward on the path to complex systems of skyrmions." One example would be new, extremely small and highly efficient storage media. Science fiction? Far from it! *rb*

Nature Materials, 15, 501-506, 2016 (DOI: 10.1038/nmat4593): Observation of room-temperature magnetic skyrmions and their current-driven dynamics in ultrathin metallic ferromagnets; S. Woo et. al.
Nature Physics, 13, 170-175, 2017 (DOI: 10.1038/nphys4000): Skyrmion Hall effect revealed by direct time-resolved X-ray microscopy; K. Litzius et. al.

THE SHORT WAVE

In experiments at HZB, an international team of researchers has succeeded for the first time in producing extremely short-wavelength spin waves in a targeted manner. They did this using nano antennae made from **magnetic vortex cores**. This could one day supersede electric current as the basis for digital data storage.

In data centres, a lot of energy is expended on simply keeping the servers cool. Computers generate not only data, but also a lot of heat, which has to be removed. This heat is produced by flowing electrons overcoming the friction resulting from constantly slamming into atoms, which slows them down as the electric current is forced through the circuits and chips. Researchers are therefore looking for alternatives to a current of travelling electric charge carriers for transferring and processing digital information. One promis-ing candidate for this is spin waves, the propagation of regular excitations of electron spins through a material. Put very simply, spin can be thought of as a revolving spinning top that has been pushed sideways. Wave-like motions in the alignment of electron spins can be generated using a magnetic field that changes over time. Like an electric current, a spin wave can also convey information, but unlike an electric current, it experiences no friction from the motion of electrons. To make optimal use of spin waves in the microscopic structures of processors and memory chips, however, their wavelengths have to be incredibly small. They would have to be produced using minute magnetic field antennae, which have so far been impossible to build by conventional means.



Simplified representation of an electron spin as a revolving spinning top that has been pushed sideways and is migrating through the material as part of a spin wave.

Vortex cores as nanoscale antennae

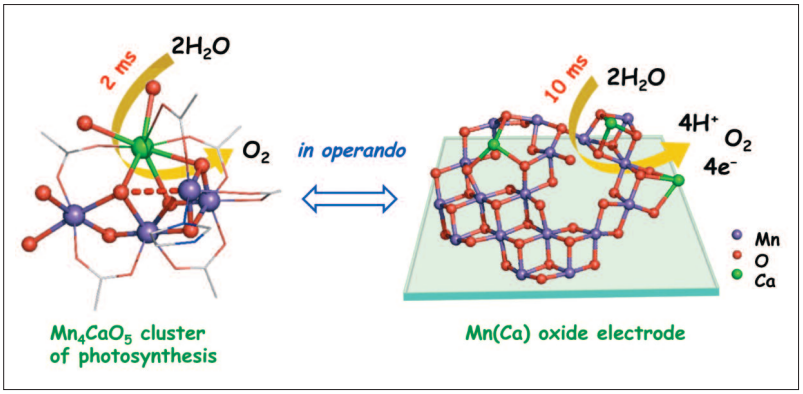
Things are different for a novel method of generating short-wave spin waves, first applied by an international team of researchers led by physicist Dr. Sebastian Wintz from the Helmholtz-Zentrum Dresden-Rossendorf. The researchers used a platelet only a few dozen nanometres thick, consisting of two thin ferromagnetic layers separated by a non-magnetic intermediate layer. “The spins arranged themselves into closed, concentric circles within the plane of the platelet – a structure known as a magnetic vortex,” Wintz explains. “However, at the centre of this vortex, within an area just a few nanometres in diameter, the spins are forced to ‘stand up’ vertically on the surface of the platelet.
When Wintz and his team colleagues excited these vortex cores with a high-frequency electromagnetic field, they acted like nanoscale antennae and generated a spin wave. At a certain thickness of the separating layer, antiferromagnetic behaviour set in. The spins in the two outer platelets tried to orient themselves in opposite directions. As a result, the distance between the “peaks” and “valleys” of the spin wave decreased further to less than 100 nanometres. On the powerful MAXYMUS X-ray microscope at BESSY II, the team was able to produce direct images of the propagation of the spin waves. The facility is operated at HZB by researchers from the Modern Magnetic Systems department of the Stuttgart Max Planck Institute for Intelligent Systems (MPI-IS). “On time-resolved X-ray images, we were able to show that the wavelength of the spin wave could be precisely tuned by selecting the excitation frequency,” says Dr. Markus Weigand, head of the workgroup X-ray Microscopy in the Modern Magnetic Systems department at MPI-IS. In their first experiments, they achieved this at frequencies of up to four gigahertz. “We are now already able to excite and observe the spin waves at much higher frequencies,” Weigand is pleased to report. This is an important step towards data processing without the wasteful heat losses in conventional computing. *rb*

Nature Nanotech., 11, 948-953, 2016 (DOI: 10.1038/nnano.2016.117): Magnetic vortex cores as tunable spin-wave emitters; S. Wintz et. al.

CATALYTIC WATER OXIDATION – MORE DYNAMIC THAN WE THOUGHT

In a joint project, scientists from Freie Universität Berlin and HZB studied how artificial photosynthesis for producing non-fossil fuels could be improved by using **manganese-based oxides** as catalysts.

In plants, algae and cyanobacteria, sunlight triggers the splitting of water molecules into molecular oxygen (O_2), protons and energetic electrons. The latter are needed for reducing CO_2 and for building carbohydrates, the indispensable "fuel" for life on earth. Catalytic water oxidation, however, is crucial not only in biological photosynthesis, but also in technologies for producing non-fossil fuels.
In biological photosynthesis, the water oxidation reaction is catalysed by a manganese complex – the Mn_4CaO_5 cluster – which is complemented by four terminal water ligands and is embedded in a protein complex known as photosystem II (PSII). The five metal ions are linked tightly via oxo bridges. The compact metal-oxygen core of this highly efficient biological catalyst is structurally similar to purely inorganic MnCa oxides. Understanding the correlations between biochemistry and inorganic oxides is therefore relevant not only to unravelling the secrets of the evolution of photosynthesis, but also to developing better synthetic catalysts for water oxidation.



In biological photosynthesis, a Mn4CaO5 cluster boosts water oxidation (left). In artificial water oxidation, an electrode coated with Mn(Ca) oxide assumes this role.

The changing Mn redox states in catalysts

PD Ivelina Zaharieva, Prof. Holger Dau and their team from Freie Universität Berlin studied amorphous, hydrated oxides at the beamlines KMC-1 and KMC-3 of BESSY II. Holger Dau explains "we were able to follow the catalysis process especially well here under real operating conditions in the medium X-ray energy range. After many preliminary experiments, we even did successful time-resolved experiments on KMC-3. We now know that structural changes that take place within a few milliseconds in the hydrous oxides are crucial, just as they are in the water splitting in biological photosynthesis."
The researchers characterised three examples of Mn-based oxides that all resemble the group of amorphous minerals known as birnessite. When these are exposed to a series of electrochemical potentials, their state and structural changes resemble those that occur in the Mn_4CaO_5 cluster of PSII in the biological water oxidation reaction cycle. The researchers furthermore discovered that the capacity to change the redox state and structure is a decisive factor for determining the catalytic activity of water-oxidising oxides. Ivelina Zaharieva explains that "applying an electric potential transforms the manganese oxide. How fast the manganese ions change redox states is crucial. The presence of a non-crystalline structure with many Mn(III) ions allows fast state changes and thus efficient water splitting." Water-oxidising Mn(Ca) oxides thus appear to be not so much "biomimetic rocks" but rather dynamic materials that are characterised by fast chemical changes of the entire oxide film – and not only on the surface. Their dynamic redox properties are crucial factors for their catalytic activity. This aspect ought to be pursued in a targeted manner in future experiments in order to deliver further insights into the catalytic mechanisms and thus to support the development of efficient catalysts for non-fossil fuel production.

ve

Energy Environ. Sci., 2016, 9, 2433 (DOI: 10.1039/c6ee01222a): Water oxidation catalysis – role of redox and structural dynamics in biological photosynthesis and inorganic manganese oxides; I. Zaharieva et. al.

MORE POWER TO WATER ELECTROLYSIS

An Israeli-German research team has developed and studied a **graphite-like layer of carbon nitride**. Containing tailored additives, the robust material will provide a much needed efficiency boost to the electrochemical production of hydrogen from water.

One key question regarding solar power is: what should we do with all the electricity that gets produced on a sunny day, but doesn't get used straight away? An elegant solution is to use the energy immediately to produce hydrogen, which can then be stored for as long as necessary, or used as a fuel, or fed into the natural gas grid. This versatile gas can be produced by splitting water with electricity (electrolysis). “One option is to use photoelectrochemical cells. This kind of cell converts the energy from sunlight into chemical energy,” says Prof. Dr. Kathrin Aziz-Lange, head of the Helmholtz Young Investigator Group “Operando Characterization of Solar Fuel Materials”.

Solar cells are the most well-known form of converting sunlight into energy. Scientists at HZB have developed an efficient cell for the electrochemical production of hydrogen from sunlight and water.

In principle, such a cell has two electrodes, one of which also acts as a photoabsorber. This absorber uses energy from sunlight to produce charge carriers that travel to the surface of the electrode, where they split the water. The trouble is, the materials used so far only convert a small percentage of solar energy into chemical energy. Also, water corrodes the materials of the system. Researchers are therefore searching intensively for new absorber materials better suited to the application.
Among those on this quest is a team of scientists from Israel and Germany. They are developing solutions working from a compound of carbon and nitrogen – a graphite-like carbon nitride. “A material has to satisfy many requirements to be used in a photoelectrochemical cell,” explains Aziz-Lange. “It has to have the right band gap to use the largest percentage of the solar spectrum possible for energy conversion.” Also, the energy bands have to be favourably positioned in the electronic structure of the material, and good electrical conductivity is needed to keep energy losses in the cell to a minimum. Also importantly, the material must be water-resistant, affordably producible, and free of toxic components.

Hot gas with additives

For large-scale production of carbon nitride photoabsorbers, one needs a deposition technique that can produce thin layers homogeneously. A group led by Israeli chemist Prof. Dr. Menny Shalom of the Max Planck Institute of Colloids and Interfaces in Potsdam therefore used the method of vapour deposition, with a twist. While the material was depositing out of a vapour onto the substrate, the Potsdam scientists added highly reactive molecules – so-called monomers – into the carbon nitride structure with the aim of improving its properties as a photoabsorber.
This was an impressive success, as Shalom’s researchers together with Kathrin Aziz-Lange and her group demonstrated. X-ray spectroscopic experiments show that the monomers are distributed perfectly evenly throughout the layer and therefore perform ideally. They found that the material absorbs sunlight over a broad spectral range, and is especially efficient in the short-wavelength region. As a result, the modified material produces about four times more electricity than a pure powder. A cell used for water electrolysis thus operates at higher efficiency and remains functional over a longer life span. As Kathrin Aziz-Lange sums up the success, “all the important properties were significantly improved.”

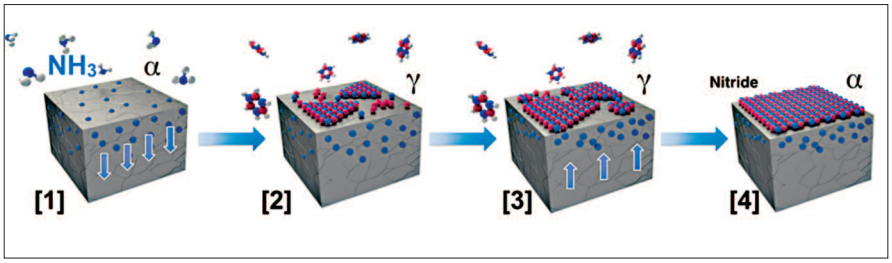
rb

Adv. Energy Mater. 2016, 6, 1600263 (DOI: 10.1002/aenm.201600263): Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design; J. Bian, L. Xi, C. Huang, K. M. Lange, R.-Q. Zhang, and M. Shalom

A SUPER-FLAT CRYSTAL FOR THE COMPUTER CHIP OF THE FUTURE

Prof. Dr. Stephan Hofmann of the University of Cambridge showed with measurements at BESSY II that **chemical vapour deposition** is suitable for producing layers of borazine one atom thick. This is an important step in the development of extremely small, high-capacity storage units.

When electronics engineers imagine the future, they tend to dream of super-flat material layers that are only one atom thick. They would use these to produce so-called "MRAM chips", for example, which would have all data accessible as soon as a computer is turned on, with no long waiting for it boot up. Or to produce micro-chips constructed much like the neurons in animals, which could therefore be assembled into energy-saving circuits. Unfortunately, it will still be some time before this miracle technology works. In 2010, André Geim and Konstantin Novoselov received the Nobel Prize for researching a super-flat material which they produced merely by pulling a piece of sticky tape off a block of graphite. This was graphene, which consists solely of carbon atoms. Although their method was worthy of the highest distinction in science, it is wholly unsuitable for high-tech application.



If ammonia first saturates the bulk of iron with nitrogen (blue), then perfect layers of h-BN (blue and red) form only one atom thick on the iron surface.

The currently preferred method of producing ultra-thin layers is therefore chemical vapour deposition, CVD. In this method, a chemical compound is vaporised and the cloud of atoms allowed to precipitate as a very thin solid layer onto a hot substrate. For example, Prof. Dr. Stephan Hofmann of the University of Cambridge vaporised the cyclic compound borazine, which consists of three nitrogen, three boron and six hydrogen atoms per molecule, to have it precipitate onto a hot iron surface where it formed the hexagonal substance boron nitride. This h-BN bears many structural similarities to graphene, which exists as a flat layer of hexagons, the corners of which are all occupied by carbon atoms. In h-BN, the hexagon corners are alternately occupied by boron and nitrogen atoms.

Pretreatment improves the process

Despite these structural similarities, there is one distinct and critical difference: graphene is an excellent electrical conductor while h-BN is not. Nevertheless, electronics engineers are still interested in materials of this kind as the switching elements of the future. MRAM could in principle consist of two magnetic layers of iron separated and thus electrically isolated by a layer of h-BN. Unfortunately, producing ultra-thin layers of these materials has proven difficult so far, especially when trying to create large surface areas or several million integrated components at a time, as the industry demands.

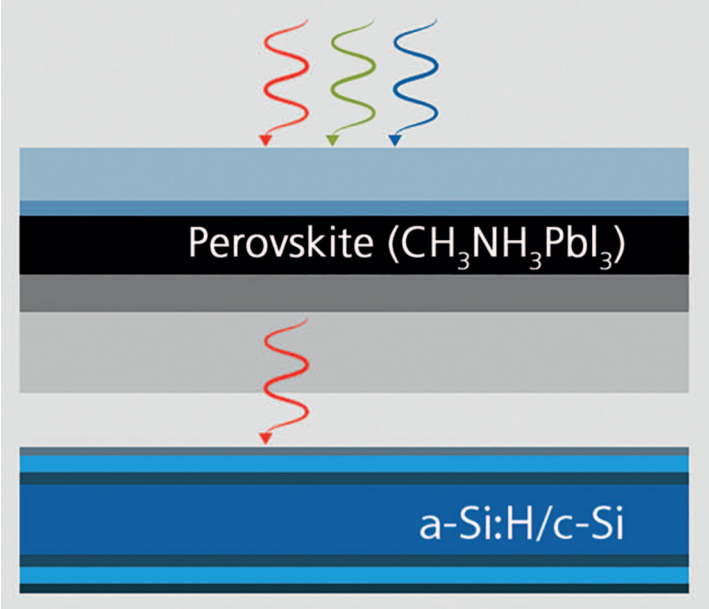
Hofmann has managed to improve the method, however, by pretreating the iron with ammonia. The nanotechnologist observed the process in situ using X-rays at a beamline of BESSY II, which Prof. Dr. Robert Schlögl of the Berlin Fritz-Haber-Institut of the Max Planck Society prepared for the researcher's high-temperature, low-pressure catalysis experiments. "Like a sponge, the iron soaks up the nitrogen atoms that were liberated from ammonia during pretreatment," Hofmann explains the results of his X-ray analysis. This saturates the bulk of the iron so that, during CVD, the nitrogen and boron atoms can only precipitate onto the substrate surface, and not be absorbed by the iron. If the researcher carefully adjusts the conditions, the atoms form the coveted h-BN in large-area layers exactly one atom thick. In addition to storage technology, this h-BN is being considered for many other applications in the electronics of the future. *rk*

Nano Letters, 2016, 16, 1250-1261 (DOI: 10.1021/acs.nanolett.5b04586): Controlling Catalyst Bulk Reservoir Effects for Monolayer Hexagonal Boron Nitride CVD; S. Caneva et. al.

HIGHER EFFICIENCY WITH A TANDEM STRUCTURE

A team of researchers from the Clarendon Laboratory at the University of Oxford and from the Institute for Silicon Photovoltaics at HZB has succeeded in developing a highly crystalline and **photostable halide material for perovskite solar cells**. This will allow so-called tandem solar cells to achieve higher efficiencies than ever before.

Currently at the centre of focus in high-efficiency solar cell research is the concept of tandem solar cells. Depending on their materials and design, solar cells produce electrical energy from different wavelengths of incident sunlight. In the tandem concept, different types of cells are stacked on top of one another in a kind of sandwich arrangement in order to optimise the overall efficiency of the tandem. The researchers led by Prof. Dr. Bernd Rech, head of the Institute for Silicon Photovoltaics, and Henry Snaith, head of the Photovoltaic and Optoelectronic Device Group at the University of Oxford, physically stacked complete perovskite cells on top of complete silicon cells. Bernd Rech explains: “we believe that in the not too distant future, the combination of established silicon technology with perovskite cells into a tandem will supersede the existing cells that have only one band gap. Such tandems allow significant increases in efficiency at little extra cost, because the perovskite cells can be produced very affordably.”



Schematic structure of a tandem solar cell made from perovskite (top) and silicon.

The material of choice: metal halide perovskite

The researchers built upon earlier results that had revealed that by tweaking the halide composition, a perovskite cell can be developed with an ideal optical band gap of ~ 1.75 electron volts (eV), and which is therefore especially efficient at converting sunlight into electricity. Until now, however, perovskites have proven relatively unstable in practice. The English–German research team successfully developed a highly crystalline and photostable material with an optical bandwidth of ~ 1.74 eV, comprising lead, the organic molecule formamidinium ($HC(NH_2)_2$), the halogens iodine and bromine, and caesium, the full formula of which is $([HC(NH_2)_2]_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})_3$. The cells produced with this perovskite achieved more than 17 per cent power conversion efficiency over small surface areas. Combining these cells with a silicon cell to make tandem cells allows a total efficiency of nearly 20 per cent to be reached. Based on realistic assumptions regarding possible improvements, the maximum efficiency attainable by such a tandem is expected to be around 30 per cent.

A whole set of challenges

Most photovoltaic cells based on metal halide perovskites are made from organic–inorganic trihalide perovskites. These, however, have fundamental problems when it comes to band gap matching and long-term stability and therefore do not satisfy the international standards for commercial solar cells.

By modifying the material composition, the research team was able to eliminate the phase instability region between iodide and bromine entirely, namely by partially substituting the formamidinium cation with caesium. Formamidinium-caesium–based perovskites thus appear to guarantee the best structural and thermal stability. This material, with its optimum band gap, is furthermore able to produce a higher

open-circuit voltage. “No higher efficiency is possible, however, when operated as a single cell: with a larger band gap, fewer photons are namely converted into photoelectric current, and the efficiency depends on the two parameters of current and voltage,” explains Lars Korte from HZB. “In the tandem cell, however, this is not a problem anymore because the photons that go unused in the perovskite cell are ‘passed on’ to the silicon cell, and so contribute to its photoelectric current. When the right band gap is chosen, the total efficiency of the tandem increases because thermalisation losses are reduced.” Under standard test conditions, the current-voltage characteristic of the best perovskite solar cell delivered an open-circuit voltage of 1.2 V and an energy conversion efficiency of 17.1 per cent. The potential applicability of the new perovskite composition in a tandem architecture was demonstrated with semi-transparent perovskite solar cells that together with silicon heterojunction cells, achieved a total efficiency – the sum of the individual cell efficiencies – of 19.8 per cent. Spectral resolution of the external quantum efficiencies of the two single cells in this tandem, however, still revealed clear optical losses, which must be reduced by further component optimisations.

The tandem solar cell has a future

Against this background Bernd Rech summarises that “given the continuous tunability of the perovskite band gap, the tandem cell can be optimally tuned to the solar spectrum.” An efficiency of up to 30 percent can be expected if the system is further optimised. The tunability over the entire visible spectrum will generally have a positive effect on the colour tunability and optimisation of perovskites for light-emitting diode (LED) applications. The benefits of this research thus extend far beyond the field of pure photovoltaics.

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Science, Vol. 351, Issue 6269, pp 151-155 (DOI: 10.1126/science.aad5845): A mixed-cation lead mixed-halide perovskite absorber for tandem solar cells; D. P. McMeekin, G. Sadoughi, W. Rehman, G. E. Eperon, M. Saliba, M. T. Hörantner, A. Haghighirad, N. Sakai, L. Korte, B. Rech, M. B. Johnston, L. M. Herz, and Henry J. Snaith

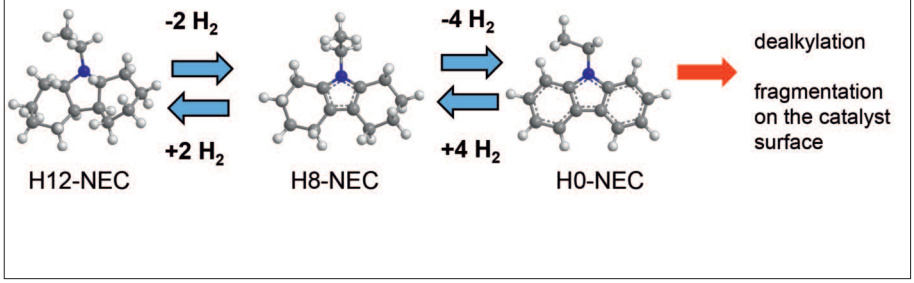
PLATINUM CATALYST FOR HYDROGEN CARS

A team of researchers from Friedrich-Alexander-Universität Erlangen-Nürnberg and the Helmholtz-Institut Erlangen-Nürnberg for Renewable Energies studied the processes occurring inside a platinum catalyst at BESSY II. This catalyst can be used to bind hydrogen into **liquid carrier materials**, which could pave the way to the efficient use of hydrogen in vehicles.

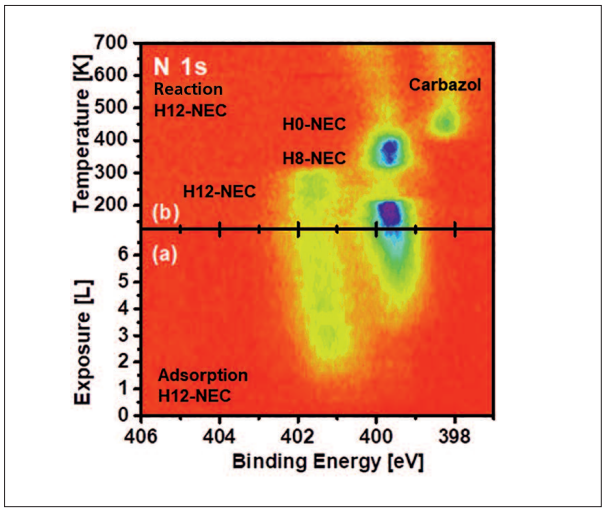
Hydrogen is still considered the most promising energy carrier for future mobility solutions; it can be produced directly from solar or wind energy and offers many of the advantages that petrol, diesel and kerosene do. Hydrogen produced by electrolysis is not only an important raw material for the chemicals industry – at an annual turnover of 60 million tonnes – but also a coveted energy carrier. In a fuel cell, it can be combined with oxygen from the air to re-form water and at the same time generate electricity that could replace wind energy during calm conditions, or drive the motor of an electric car. On top of that, one kilogram of hydrogen stores about as much energy as three kilograms of petrol or diesel. Unfortunately, its very high energy density applies more to its weight than its volume: at sea level, one kilogram of hydrogen would require a tank of more than 11,000 litres capacity. Obviously, none of us wants to drag a giant balloon tank behind our car, and so gaseous hydrogen forfeits its candidature as a transportation fuel. We could liquefy the gas by cooling it to extremely low temperatures below minus 250 degrees Celsius, or squeeze it into a manageable volume at extremely high pressures. The trouble is, any tank built with all the necessary cooling equipment or a pressure vessel strong enough to hold the hydrogen would be many times heavier than a petrol tank. Then, there are the problems that liquid hydrogen slowly but surely evaporates and that compressed hydrogen gas tends to escape through even the tightest of hulls over time.

Liquid hydrogen carriers

These disadvantages can be avoided by using liquids such as N-ethylcarbazole (NEC) or dibenzyltoluene (DBT). In the presence of a catalyst at low temperatures, these two materials positively soak up hydrogen and thus become energy stores in the form of oily liquids that strongly resemble a diesel fuel, and behave much like one as well. The researchers call these substances "liquid organic hydrogen carriers", or LOHC. "That means we can continue to use the existing infrastructures such as service stations and tankers for handling hydrogen stored in LOHC systems," explains Prof. Dr. Peter Wasserscheid. As the founding director of the Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), the process engineer wants to unite the efforts in this field at Jülich, HZB and Friedrich-Alexander-Universität Erlangen-Nürnberg.



In two steps, the NEC carrier first releases four and then another eight hydrogen atoms. Higher temperatures cause a side-chain to break off the liquid hydrogen carrier, thus destroying it.



This colour-coded illustration shows the process of hydrogen-loaded NEC first releasing four and then another eight hydrogen atoms, and then ultimately being destroyed by the loss of a side-chain.

We could one day be filling hydrogen-loaded NEC or DBT into the tanks of our fuel-cell cars, which would then extract the hydrogen from the liquid. This extraction would take place in a catalytic converter featuring a platinum catalyst. It would consume a small amount of energy but, on the whole, LOHCs still fare much better than the other two options of direct hydrogen liquefaction or high-pressure storage and their associated drawbacks.
"The catalytic converter, however, is still something of a bottleneck for vehicle applications," physicochemist Dr. Christian Papp of Universität Erlangen-Nürnberg admits. While the platinum catalyst causes NEC and DBT to release their bound hydrogen very well, the overall converter design still has to be made lighter and more compact. Such improvements become easier to make as the researchers gain a better understanding of how the catalyst actually helps release the hydrogen.
Thus, we regularly find Christian Papp loading his experimental system onto a truck and transporting it from his lab in Erlangen to an open port at the Berlin synchrotron BESSY II. The electron beam there delivers such a high photon density that the researcher can observe the processes occurring on a platinum catalyst one square centimetre wide and three millimetres thick at high detail in only a few seconds. "With BESSY II we can, so to speak, record live pictures from the surface of the catalyst over very short intervals," the researcher explains.

Tracing the route travelled by the hydrogen atoms

As the BESSY II data reveal, it turns out that hydrogen-loaded NEC releases its hydrogen in two distinctly separate steps. The NEC molecule consists of two rings of six carbon atoms each (two six-rings), where two carbon atoms from each ring combine with a nitrogen atom to form a five-ring that "welds" the two six-rings together. In the first step, the hydrogen-loaded NEC releases four hydrogen atoms from this middle five-ring. High temperatures then give enough of an energy push to release another eight hydrogen atoms in total from the two six-rings. Still higher temperatures then split a side-group off the NEC, destroying the liquid energy carrier, which suddenly turns solid. Thanks to these detailed images, the researchers can continue to tweak the catalyst and thus optimise it further for use in motor vehicles.

rk

Acc. Chem. Res. 2017, 50, 74–85 (DOI: 10.1021/acs.accounts.6b00474): Liquid Organic Hydrogen Carriers (LOHCs): Toward a Hydrogen-free Hydrogen Economy; P. Preuster, C. Papp, and P. Wasserscheid

SELF-HEALING IN SPACE

A German-Italian research team studied organic-inorganic **solar cells made of perovskites** under space-like conditions at HZB. They are highly robust against radiation damage, and resulting defects even self-repair. This makes them promising candidates for use in space missions.

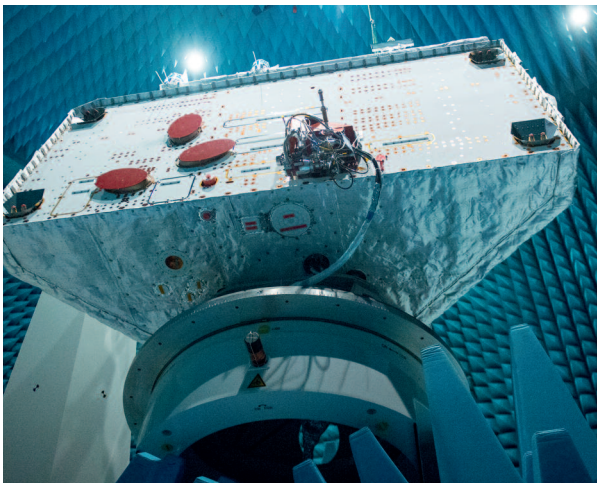
Far above our heads, out in space, the conditions are brutal. Not only for astronauts, but also for the solar cells that are supposed to power satellites and space probes with solar electricity. The problem, above all else, is the high-energy cosmic radiation, a constant barrage of high-energy particles – for example protons and alpha particles, the nuclei of hydrogen and helium atoms – relentlessly eating away at the materials. Measurements have shown that at times, several trillion particles can bombard each square millimetre of the PV cell surface in a day. The resulting material degradation impairs the cell's capacity to convert sunlight into electricity.

"So far, mostly silicon solar cells or tandem solar cells made from gallium-indium phosphide have been used on space flights," says Felix Lang, researcher at the HZB Institute for Silicon Photovoltaics. Tandem solar cells stand for a high degree of efficiency, but unfortunately they are particularly sensitive to cosmic radiation. "On some satellite missions, the solar cells had already lost around ten percent efficiency after one month," Lang reports. Up to now, space engineers have steered clear of other solar cell materials such as CIGS, which stands for copper-indium-gallium diselenide. While CIGS is namely more resistant to cosmic radiation than other semiconductors, its efficiency is simply too low.

Artificial cosmos in a proton accelerator

The solution comes in the form of certain perovskite crystals, as Lang and research colleagues at HZB and the University of Salerno, Italy, were to discover. The scientists used a proton accelerator on the Lise Meitner Campus in Berlin-Wannsee, which is also frequently used for treating tumour patients, in order to study the effect of energy-charged hydrogen nuclei on perovskite cells. The radiation in this facility is similar to the high-energy particle flux from the cosmos.

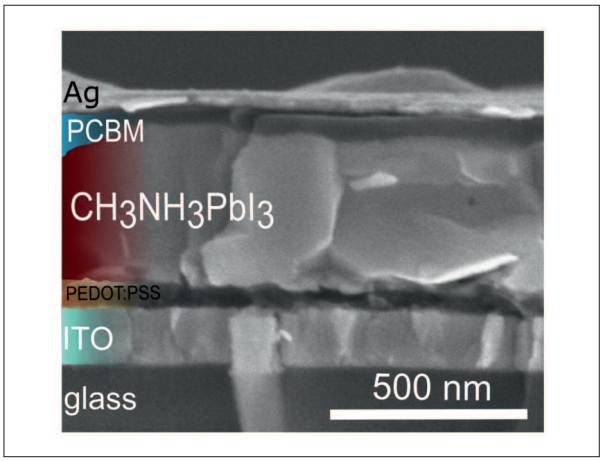
The researchers fired protons of various intensities at a perovskite solar cell over a period of ten days. During the process, they measured the changes in physical characteristics, from which the efficiency of the cell can be deduced. The material of the test cell comprised a complex chemical mixture of nitrogen, lead, iodine and methyl groups – a so-called hybrid perovskite. To provide comparative values, the researchers also subjected a conventional silicon solar cell to the same degradation conditions. "Because bombarding with protons creates radioactive elements, we had to set up an autonomous measuring system in the accelerator complex and observe the measurements through a camera," Lang reports.



The space probe BepiColombo in the European Space Research and Technology Centre (ESTEC) in Noordwijk, Netherlands, is set to embark on its journey to Mercury in 2018. Guaranteeing a reliable power supply in space puts extremely high demands on the solar cells.

Witnessing self-healing powers

So, what were the results? "The efficiency drop in the perovskite was far lower than in the reference silicon sample," says Lang. In fact, the perovskite can withstand radiation doses so high that silicon solar cells completely cease to function. What is more, after the radiation was turned off, the efficiency of the proton-irradiated perovskite solar cell even restored itself over the course of a few days. The defects, which the researchers presume are the result of chemical bonds being broken between carbon or nitrogen atoms and water molecules, thus gradually "heal".



Scanning electron micrograph of a solar cell with a thin layer of perovskite in the middle. At the core is a layer of the material CH3NH3PbI3 around 400 nanometres thick.

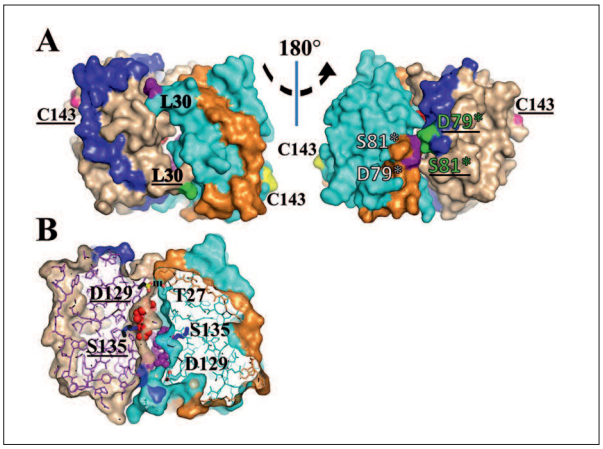
"This makes perovskite solar cells ideally suited to use on satellites and spacecraft," Lang believes. Not only are they resistant to radiation, but some can also reach a high efficiency of above 20 percent. Lang's idea is to combine a thin layer of a suitable perovskite with CIGS. Such a tandem solar cell would make especially good use of the solar spectrum to generate electricity. These robust cells could one day even be used not only in space, but also for applications down here on earth, as Lang imagines: rugged radiation or light sensors, for example, or to produce electricity in large-scale solar parks in the contaminated areas around Chernobyl or Fukushima that cannot be inhabited in the foreseeable future. *rb*

Adv. Mater. 2016, 28, 8726–8731 (DOI: 10.1002/adma.201603326): Radiation Hardness and Self-Healing of Perovskite Solar Cells; F. Lang, N. H. Nickel, J. Bundesmann, S. Seidel, A. Denker, S. Albrecht, V. V. Brus, J. Rappich, B. Rech, G. Landi, and H. C. Neitzert

PROGRESS IN THE FIGHT AGAINST THE ZIKA VIRUS

Scientists from the University of Lübeck elucidated the structure of a key protein in the **Zika virus** pathogen by performing experiments at BESSY II. This is an important first step towards developing an effective drug against the dangerous virus.

Because the Zika virus causes severe malformations of the brain in unborn children, the World Health Organisation, WHO, declared a state of "Public Health Emergency of International Concern" on 1 February 2016. At the time, scientists around the world were already working fervently to discover how a certain active agent worked – one that inhibits a key protein in the Zika virus without which the pathogen cannot propagate. In this race among the world's top researchers, Prof. Dr. Rolf Hilgenfeld of the University of Lübeck and his colleagues ultimately found themselves a step ahead. At the end of March 2016, nearly two months after the WHO had put the world on alert, experiments performed at the electron storage ring BESSY II delivered the first data for describing the rough structure of the inhibited protein. The researchers then presented even more data on this structure to the world on 7 July 2016, obtained from detailed analyses at the Deutsche Elektronen-Synchrotron DESY. This has paved

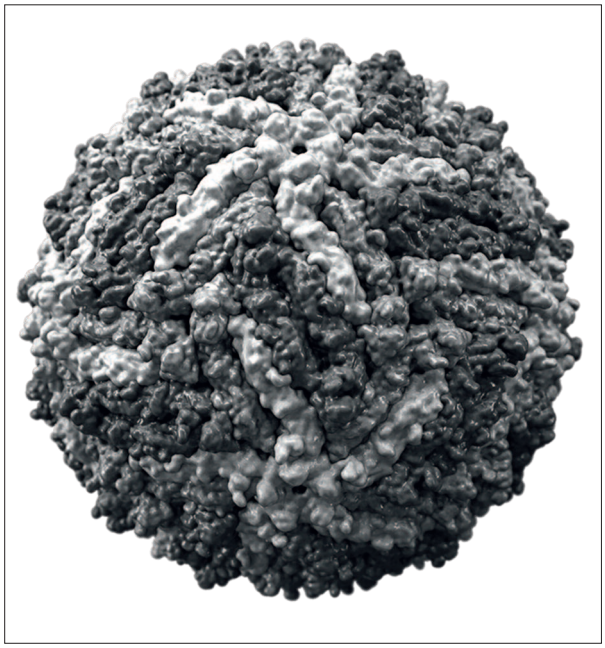


View of a crystal of the Zika virus enzyme responsible for reproduction of the dangerous virus, after the enzyme has been blocked by boronic acid. Figure A shows the front and back of the crystal; Figure B shows a cross section.

the way towards developing drugs against the insidious infectious disease.
Researchers are concentrating on antiviral drugs against Zika for a valid reason: while a good vaccine could prevent an infection, it seems we are still a long way off from developing one. In the meantime, physicians would welcome drugs that at least incapacitate the virus. To develop these drugs, researchers such as Rolf Hilgenfeld first have to find out what they are up against.
Zika viruses are classified under the flaviviridae, making them related to the viruses that cause dengue, West Nile and yellow fever, and even the pathogen behind European tick-borne (meningo)encephalitis, TBE. Mosquitos and ticks transmit these viruses to humans and animals. While the genetic material of practically all life forms on earth consists of two intertwined strands of nucleic acids, called “DNA”, the genetic material of flaviviruses consists of a single strand of nucleic acids, which molecular biologists call “RNA”.

Reproduction successfully halted

When animals, plants and bacteria produce proteins – the building blocks of cells – they first create a copy, or “transcription”, of their DNA in the form of a single RNA strand, which then serves as a template for assembling the proteins. Flaviviruses can spare this transcription step because they already use RNA as their genetic code. Once a Zika virus has infected a cell, the cellular machinery starts building a giant protein conglomerate according to the virus’s template. Next, an enzyme also introduced by the virus cuts this enormous molecule down into the ten proteins that make up the Zika virus itself.
If a drug could shut down this latter viral enzyme, known as a “protease”, the protein conglomerate would no longer be cut into segments. Then, no new viruses could form and the infection would be halted – at least in theory. In practice, Prof. Dr. Christian Klein of the University of Heidelberg has indeed developed an agent based on boronic acid that reliably shuts down the Zika protease. Unfortunately, this “boronate inhibitor” cannot be used as a drug because there is no way to transport it to the site of infection in the body.
Nevertheless, analysing how this inhibitor blocks Zika virus protease is significant because the knowledge should allow researchers to develop other agents that can be turned into drugs which deactivate the virus enzyme in similar fashion. In order to learn more, Rolf Hilgenfeld and colleagues therefore produced the Zika protease in the bacterium Escherichia coli. The researchers were surprised to discover that the Zika enzyme operates considerably faster and more efficiently than its homologues from the dengue, yellow fever and West Nile viruses.
After inhibiting the Zika virus enzyme with boronic acid, the researchers produced crystals of the enzyme in preparation for X-ray analysis. Normally, beamtime for an experiment of this kind would have to be applied for long in advance. Given the importance and urgency of the issue, however, Dr. Manfred Weiss, head of the HZB research group Macromolecular Crystallography (NP-GMX) pulled every string to expedite Rolf Hilgenfeld’s experiments for determining the X-ray crystal structures at BESSY II. At the end of March 2016, the researchers obtained the first data on a rough structure of the Zika virus protease–boronate complex. From this data, they were able to elucidate structures a mere 0.4 nanometres in size, in other words less than a millionth of a millimetre in size.
They then worked intensely to produce even better crystals for their next studies in April 2016 at DESY in Hamburg, also operated by the Helmholtz Association, and were able to bring out details at a higher resolution of 0.27 nanometres. From these studies, they discovered that boronic acid blocks a serine amino acid that sits in exactly the site of the Zika virus protease which is responsible for breaking down the giant protein molecule into ten Zika virus proteins. Armed with this knowledge, Rolf Hilgenfeld is now searching for substances that block the protease at the same site and which – unlike boronic acid – can be developed into drugs. If he is successful, then the threat posed by Zika viruses could soon be diminished. *rk*



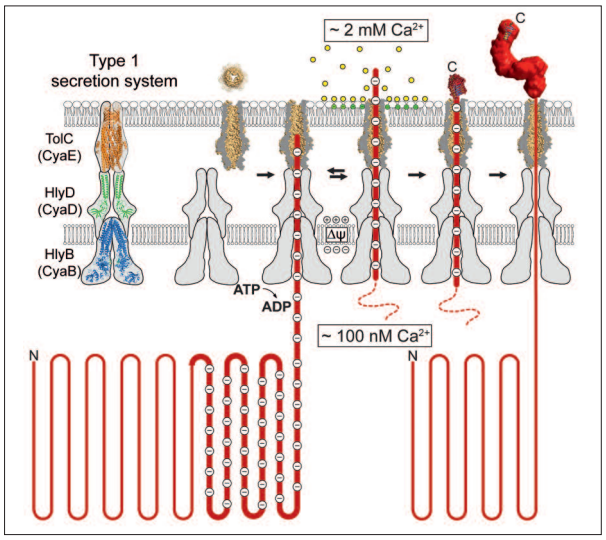
3D reconstruction of the Zika virus. It mainly attacks skin cells and neuronal stem cells. Impaired brain development of children in the womb most likely occurs due to the infection of embryonic neural stem cells.

Science, 353, pp. 503-505, 2016 (DOI: 10.1126/science.aag2419): Crystal structure of Zika virus NS2B-NS3 protease in complex with a boronate inhibitor; J. Lei, G. Hansen, C. Nitsche, C. D. Klein, L. Zhang, and R. Hilgenfeld

WEAKEN, DON'T KILL

Scientists from the Institute of Microbiology of the Academy of Sciences in Prague experimented at BESSY II to observe processes occurring in the **whooping cough pathogen *Bordetella pertussis***. Their findings reveal a new approach to the development of effective drugs.

The medical profession is facing a high-risk problem in hospitals: a constantly growing number of micro-organisms are rendering the best weapons of modern medicine useless. Prof. Dr. Peter Sebo, an infection biologist from the Institute of Microbiology of the Czech Academy of Sciences in Prague, summarises the reason for this trend: "Antibiotics kill bacteria. Accordingly, the pressure on these organisms to neutralise the active agents is very high." Newly developed antibiotics work excellently for the first few years. However, at some stage microorganisms appear that can survive this treatment. These resistant strains then prevail over all others. Presently, many thousands of people



Insight into the whooping cough pathogen: to defend itself against macrophages, the bacterium secretes adenylate cyclase – namely by its "C-end" first, which then folds in the presence of calcium. New drugs could prevent this folding and thus effectively cripple the whooping cough pathogen.

die each year from antibiotic-resistant germs. Their chances would be much better by using drugs that put the pathogens under less pressure to survive. Instead of directly killing the microbes, these drugs would merely weaken their ability to cause disease. To achieve this, one must fully understand the process of infection. Peter Sebo and his colleagues are therefore studying the whooping cough pathogen *Bordetella pertussis*. When this bacterium gets into the respiratory tract, the body's immune system tries to fight off the invader using "macrophages" (Greek for "big eaters"). The whooping cough pathogen, however, produces its own counter-defence in the form of the toxin adenylate cyclase. When this protein penetrates into the macrophages, it shuts them down.

Preventing adenylate cyclase from folding

Peter Sebo is therefore interested to learn more about this adenylate cyclase, for example how the bacterium secretes the enormous biomolecule through its outer envelope. His colleague Ladislav Bumba and others discovered that the calcium normally found abundantly in tissue plays a key role in the process. X-ray analyses at the synchrotron BESSY II ultimately revealed important steps in the process. Adenylate cyclase, like other proteins, is a long chain of various amino acids. This chain is transported through the bacterial envelope as a long, strung-out molecule by what the biochemists call its "C-end" first. Calcium not only greatly accelerates this process, but is also instrumental in the final folding of the protein. The C-end of adenylate cyclase thus becomes a thick lump, which would have been too big to be transported through the envelope. While it is now blocked from re-entering the bacterium, adenylate cyclase can only be "eaten" by the macrophages when in this form.
If the researchers merely swap two amino acid components near the C-end, then its folding is disrupted, and the adenylate cyclase becomes far less effective at shutting down the macrophages. "With this modification, the population of whooping cough bacteria would have to be ten times greater for a successful infection," Peter Sebo explains. Armed with this knowledge, the search can now begin for agents that prevent the folding of adenylate cyclase and thus reduce the infectiousness of the bacterium. *rk*

Molecular Cell, 62, pp. 47-62, 2016 (DOI: 10.1016/j.molcel.2016.03.018): Calcium-Driven Folding of RTX Domain beta-Rolls Ratchets Translocation of RTX Proteins through Type I Secretion Ducts; L. Bumba et. al.

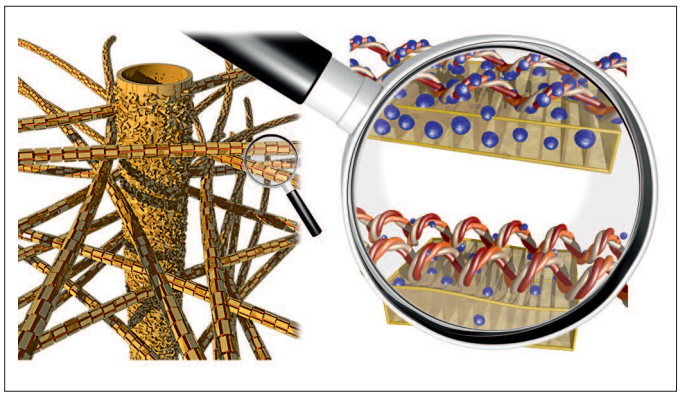
WHAT MAKES TEETH STRONGER THAN ANY FILLING

Scientists from Charité Universitätsmedizin Berlin studied the **nanostructure of dentin** in experiments at BESSY II and discovered the reason behind its extraordinary strength. Their findings provide clues as to how to develop better fillings.

In humans, teeth come into contact almost 5,000 times per day under normal use. In spite of this, and although we often apply great forces while we chew, it is surprisingly rare for healthy teeth to break. It is widely accepted that the structure of teeth makes them tough, where an inner core known as dentin supports the hard outer enamel cap. The secret to this remarkable toughness lies in the finer details of their structure. Dentin is a bone-like substance composed of mineral nanoparticles, collagen and water. While both enamel and dentin are composed of the same mineral called carbonated hydroxyapatite (cHAP), dentin represents a complex nanocomposite material. It consists of inorganic cHAP nanoparticles embedded in an organic matrix of collagen protein fibres. A group of researchers, led by Dr. Jean-Baptiste Forien and Dr. Paul Zaslansky from Charité's Julius Wolff Institute, had previously shown that residual stress in dentin contributes to the high load-bearing capacity of this biological structure.

Interplay between nanoparticles and collagen fibres

Compression stress found within the material can explain why damage or cracks in the enamel do not extend catastrophically into the dentin bulk. As part of the new findings, Dr. Zaslansky's team used samples of human teeth to measure how nanoparticles and collagen fibres interact under humidity-driven stress. "It was the first time we succeeded in precisely determining not only the lattice parameters of the cHAP crystals contained within the nanoparticles, but also the spatially varying size of the nanoparticles themselves. This also allowed us to establish the degree of stress they are generally able to withstand," says Zaslansky. In order to gain insights into the performance of the nanostructures involved, the researchers conducted laboratory experiments and measurements at HZB's synchrotron radiation source BESSY II, a device that produces radiation frequencies ranging from terahertz to hard X-rays.
As part of their experiments, the researchers increased the compressive stress inside the dentin samples. The samples were also dried by heating them up to 125 degrees Celsius. This caused the collagen fibres to shrink, leading to huge stress being exerted on the nanoparticles. The ability to withstand forces of up to 300 Megapascal is equivalent to the yield strength of construction grade steel, and is comparable to 15 times the pressure exerted during the mastication of hard food, which usually remains well below 20 Megapascal. Heat treatment did not lead to destruction of the protein fibres, suggesting that the mineral nanoparticles also have a protective effect on collagen.
Analysis of the data also revealed a gradual reduction in the size of the cHAP crystal lattices as one moves deeper into the tooth. "Tissue found near the dental pulp, which is formed during the later stages of tooth development, contains mineral particles that are made up of smaller cell units," explains Zaslansky. The nanoparticle length shows the same trend, with the mineral platelets situated near bone on the outer parts of the root measuring approximately 36 nanometres in length, while those found near the pulp are smaller, only 25 nanometres long.



Normally, collagen fibres are hydrated (right picture above). Heat treatment leads to dehydration (right picture below) and makes the fibres shrink. This leads to extreme pressure on the nanoparticles.

Inspiration for novel dental restoration materials

Such a design could be used as a model system for new material developments, for example when designing novel dental restoration materials. "Dentin's morphology is considerably more complex than we had expected. Enamel is very strong, but also brittle. In contrast, the organic fibres

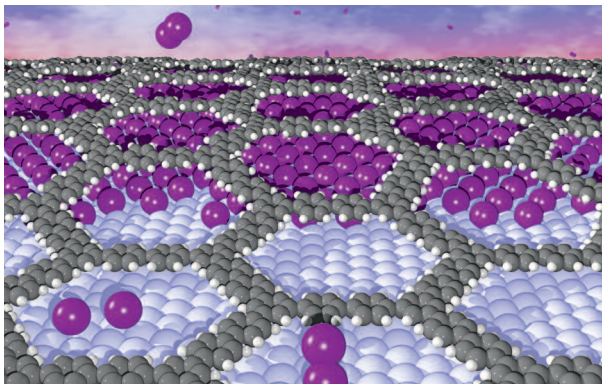
found in dentin appear to exert exactly the right pressure on the mineral nanoparticles that is required to increase the material's repetitive, cyclic load-bearing capacity", the scientists argue. At least, this is the case as long as the tooth remains intact. Bacteria that cause dental decay soften and dissolve the mineral, and produce enzymes that destroy collagen fibres. Teeth become more fragile as a result and can then break more easily. The findings of this study are also of interest to practicing dentists. Dr. Zaslansky explains "our findings highlight an important reason for doctors to keep teeth moist during dental procedures, such as when inserting dental fillings or installing crowns. Avoiding dehydration may very well prevent build-up of internal stresses, the long-term effects of which remain to be studied." *arö/Charité*

Chemistry of Materials, 2016, 28 (10), pp 3416–3427 (DOI: 10.1021/acs.chemmater.6b00811): Water-Mediated Collagen and Mineral Nanoparticle Interactions Guide Functional Deformation of Human Tooth Dentin; J.-B. Forien et. al.

SOFT DECOUPLING OF ORGANIC MOLECULES ON METAL

An international team has discovered an elegant way to decouple organic nanosheets grown on metal surfaces. This opens up new ways to transfer organic **nanostructures from metal surfaces** onto more suitable substrates for molecular electronics.

Specific organic molecules – typically on reactive metallic surfaces – can interlink via chemical bond formation into extended nanostructures. Highly stable two-dimensional molecular networks can be grown in this manner. However, these networks then also adhere to the metallic support, which strongly influences their properties. To make use of these kinds of organic networks in molecular electronics, for instance, the metal would have to be laboriously removed.



Die Grafik veranschaulicht, wie Jodatome (lila) zwischen das organische Netz und die metallische Unterlage wandern und so die Haftung reduzieren.

Now a team headed by Markus Lackinger at the Technical University Munich and the Deutsches Museum together with partners at other universities in Germany and Sweden have discovered an elegant way to reduce the adhesion between the network and the metal. They simply exposed the networks bound to the metal to iodine vapour. "After the networks had been synthesised on a silver surface, we used iodine vapour. We hoped iodine would embed between the organic layer and the metal", explains Lackinger. To do this, they investigated a nanosheet consisting of interlinked phenyl rings (polyphenylene) on a silver surface. The iodine actually migrated beneath the interlinked phenyl rings to form an atomically thin interlayer on the metal surface. After the intercalation of the iodine, measurements at BESSY II proved that the molecular network behaved almost as if it was detached. The strong influence of the metal was reduced.

Application: new transfer techniques

These results could be advantageous for future applications. "Molecular nanosheets do not grow on any surface. For this reason, we have to develop transfer techniques. Then we could fabricate the networks on metal surfaces and subsequently transfer them over to other surfaces that are more suitable for molecular electronics. Being able to mitigate the adhesion with an iodine interlayer is possibly a first step in this direction", explains Lackinger. *arö*

Angewandte Chemie, Int. Ed., Vol. 55, Issue 27, pp 7650-7654 (DOI: 10.1002/anie.201600684): Post-Synthetic Decoupling of On-Surface Synthesized Covalent Nanostructures from Ag(111), A. Rastgoo-Lahrood et. al.

NEW HZB INSTITUTE FOR ENERGY MATERIALS

DR. CATHERINE DUBOURDIEU HAS BEEN HEADING THE INSTITUTE "FUNCTIONAL OXIDES FOR ENERGY-EFFICIENT INFORMATION TECHNOLOGY" SINCE APRIL 2016.

The HZB has boosted its energy materials research and set up a new institute. Through the Helmholtz Recruitment Initiative, the HZB has gained renowned researcher Catherine Dubourdieu as Institute Director. In the newly established institute "Functional Oxides for Energy-Efficient Information Technology", the physicist is researching into thin films of metal oxides that make especially promising candidates for information technologies of the future. After holding posts in France and the USA, Dubourdieu worked at the institute "Nanotechnologies de Lyon" of the CNRS before she followed the request to work at HZB. Dubourdieu is an internationally recognised expert in her field of functional oxides. These are thin films of metal oxides that are considered an especially promising class of material for energy-efficient components. Thin films of different metal oxides stacked together into "sandwich" structures exhibit entirely new mechanical, optical and electromagnetic properties.

The synchrotron source BESSY II offers Catherine Dubourdieu a diverse range of instruments for her energy material research. These include tools for analysing processes in energy materials *in situ* and *in operando*. Besides her own synthesis and analytical chamber in the Energy Materials In situ Laboratory (EMIL) she is also involved in establishing the Helmholtz Energy Materials Foundry (HEMF) at the HZB. There, they are creating ultra-modern laboratories for material synthesis, which will also be available for use by external researchers.

HZB SETS UP THE HELMHOLTZ INNOVATION LAB HYSPRINT

NEW COMBINATIONS OF MATERIALS AND PROCESSES IN ENERGY APPLICATIONS ARE THE GOAL.

The Helmholtz Association is supporting a total of seven Helmholtz Innovation Labs in order to strengthen the transfer of research results to the applications domain. The association is making about twelve million euros available until 2020 for setting up and operating the Innovation Labs. The HZB proposal HySPRINT was selected in a competitive process from a field of 27 applications. HySPRINT stands for "Hybrid Silicon Perovskite Research, Integration & Novel Technologies". It will focus on hybrid materials and components based on silicon and perovskite crystals able to be employed for energy conversion in photovoltaics as well as for solar hydrogen production. "We intend to further develop silicon hybrid technology, liquid-phase crystallisation of silicon, nano-print lithography as well as the implementation of prototypes by means of 3D techniques for micro-contacts in cooperation with industrial partners – and demonstrate the potential for industrial-scale production", says Professor Bernd Rech from the HZB Institute for Silicon Photovoltaics and provisional scientific director of the HZB. The Helmholtz Association is supporting the project with 1.9 million euros, with additional contributions from HZB itself as well as from industry.

HySPRINT
Helmholtz Innovation Lab

ERC ADVANCED GRANT FOR PROF. FÖHLISCH

The European Research Council promotes unconventional, trailblazing research and supports outstanding researchers. Alexander Föhlisch holds a joint appointment at the Institute for Physics and Astronomy of the University of Potsdam and is head of the HZB Institute Methods and Instrumentation for Synchrotron Radiation Research. With the ERC Advance Grant, he receives a total of 2.5 million euros over a five-year period to support his work on highly selective methods of detection using synchrotron light and X-ray lasers. The new research project is named "Excited-State Dynamics from Anti-Stokes and Non-Linear Resonant Inelastic X-Ray Scattering" (EDAX). Under this programme, Prof. Föhlisch will study how chemical reaction pathways and phase-transition behaviour can be probed using novel X-ray spectrographic methods. These will serve as a foundation for efficient energy conversion and future energy-efficient information technologies.

TWO YOUNG INVESTIGATOR GROUPS FOR PEROVSKITES

DR. STEVE ALBRECHT AND **DR. ANTONIO ABATE** ARE SEARCHING TO PROLONG THE LIFESPAN OF PEROVSKITE SOLAR CELLS.

With funding from the Federal Ministry of Education and Research, Steve Albrecht is researching a more sustainable energy supply for the future.

Dr. Antonio Abate is setting up a Helmholtz Young Investigator Group at HZB. He intends to increase the life span of perovskite solar cells.

Steve Albrecht has headed the BMBF Young Investigator Group "Perovskite Tandem Solar Cells" at HZB since mid-2016. The German Federal Ministry of Education and Research (BMBF) is providing him with five years of funding to set up his own research team. There is also further funding for laboratory expansions. Steve Albrecht has been working on photovoltaics since he wrote his diploma thesis. He completed his doctorate in 2014 at the University of Potsdam on the subject of organic solar cells. Directly after that, he moved to HZB, where he has been researching hybrid tandem solar cells ever since. He now aims to make advancements in perovskite technology with the establishment of his own workgroup. "While silicon solar cells have a high efficiency and make up about 90 percent of the market, their efficiency cannot be significantly increased any further. But if we combined silicon with other materials, then we could increase efficiency and lower costs," the junior researcher explains. Steve Albrecht is now combining silicon with perovskite materials to make tandem solar cells. The advantage is that together, these materials can convert more energy from sunlight into electricity than either material alone. However, perovskites are not yet stable enough to last the 20 years a PV system is supposed to.

At the end of 2016, HZB announced it will boost its research on perovskite solar cells with the new Helmholtz Young Investigator Group "Active Materials and Interfaces for Stable Perovskite Solar Cells", headed by Dr. Antonio Abate. The Italian scientist, who previously worked at the University of Fribourg, Switzerland, came out on top in a highly competitive selection process of the Helmholtz Association and will now be receiving 300,000 euros per year in funding over a period of five years. Abate will be studying the materials and interfaces of perovskite solar cells in order to improve their long-term stability. Prof. Dr. Bernd Rech, the provisional Scientific Director of HZB, said: "Perovskite solar cells are one of the most promising material classes to be discovered in the last few years. HZB is already working actively in this field. We are very pleased to have the reinforcement of Antonio Abate and the new group he is putting together. This will help us to achieve rapid results in the field." *kk/sz*

NEW HELMHOLTZ YOUNG INVESTIGATOR GROUP

DR. MATTHEW T. MAYER HAS PUT TOGETHER A HELMHOLTZ YOUNG INVESTIGATOR GROUP IN THE FIELD OF ENERGY MATERIALS RESEARCH AT HZB.

Researchers are faced with the major challenge of developing new solutions for reducing the harmful emissions of carbon dioxide into our environment. One feasible solution is to use clean energy that will convert carbon dioxide and water electrochemically into hydrocarbons such as methane, methanol and ethylene, which are important raw materials for the chemicals industry. The biggest hurdle will be improving the energy efficiency, reaction rates and yields from CO_2 catalysis.

Matthew T. Meyer, who previously worked at École Polytechnique Fédérale de Lausanne (EPFL), is searching for answers to exactly these problems. He will be receiving 300,000 euros per year over a period of five years to run his Young Investigator Group.

HZB AND ANSTO EXTEND THEIR SCIENTIFIC COOPERATION

ENERGY MATERIALS RESEARCH MUST BE PURSUED FURTHER.

The management of the two institutes at the signing of the Memorandum of Understanding for intensifying their cooperation.

The heads of HZB and the Australian Nuclear Science and Technology Organisation (ANSTO) have considerably extended the Memorandum of Understanding existing between the two institutions since 2015. Their intention is to intensify their cooperation particularly in the field of energy materials research. The memorandum comprises agreements on the exchange of personnel, advanced training, and reciprocal access to instruments located at the large-scale facilities of ANSTO and HZB. ANSTO's research hub is located near Sydney, operating a synchrotron source as well as other infrastructures including the OPAL research reactor and Australian Centre for Neutron Scattering. ANSTO will be taking over the BioRef Reflectometer for conducting research on soft matter and solid-state/liquid interfaces from the Berlin-based neutron source BER II, scheduled for shutdown at the end of 2019.
Furthermore, HZB has enhanced its collaboration with other leading Australian institutions. In summer 2016, Monash University appointed three HZB scientists from the field of energy materials research as adjunct professors. In this position, HZB scientists Prof. Dr. Klaus Lips, Dr. Alexander Schnegg and Prof. Dr. Emad Aziz are entitled to organise workshops and seminars at Monash University and to promote joint research projects.

FIRST STUDENTS FINISHED AT THE GRADUATE SCHOOL MATSEC

THE FIRST FOUR STUDENTS OF THE GRADUATE SCHOOL **MATERIALS FOR SOLAR ENERGY CONVERSION** HAVE SUCCESSFULLY DEFENDED THEIR PHD THESES.

MatSEC is the first graduate school HZB installed in 2013 under the roof of Dahlem Research School in cooperation with several universities of the region. In the summer term of 2013 and the winter term of 2013/2014, the first seven PhD students of the newly established graduate school MatSEC started their PhD at HZB.
The first four students finished in December 2016: Anna Ritscher from Technical University Berlin, and Marcel Quennet, Laura Elisa Valle Rios and Kai Neldner from Freie Universität Berlin.

The graduate school is well set for the future. "MatSEC is to be continued, but with a much broader research field," Prof. Dr. Susan Schorr, speaker of MatSEC, explains. The organisers can rely on their cooperation with other research institutes and universities in Germany and have won two new international partners from Israel: the Weizmann-Institute of Science in Rehovot and the Hebrew University in Jerusalem. Young scientists can apply now for PhD grants in MatSEC.

IMPORTANT APPOINTMENTS

Prof. Dr. Bella Lake, head of the department Quantum Phenomena in New Materials, accepted a W3 professorship in a joint appointment procedure of Technische Universität Berlin and HZB. She accepted the position on the first of December 2016.

Yan Lu, group leader at the Institute for Soft Matter and Functional Materials, accepted the position of a W2 professorship at the University of Potsdam.

Kathrin Aziz-Lange, head of the Helmholtz Young Investigator Group "Operando Characterization of Solar Fuel Materials" was appointed junior professor at the University of Bielefeld on the first of November 2016.

Marcus Lörgen, head of the department "Precision Gratings", received a W2 professorship at the HTW Berlin, which he took up on 1 February 2017.

Organisation Chart HZB

Date September 2017, Rev. September 19th, 2017 GB

HZB Helmholtz Zentrum Berlin

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(German Federation and State of Berlin)

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(Chairman: Dr. K. E. Huthmacher)

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Chairwoman: Prof. Dr. S. Schorr

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Board of Directors

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Prof. Dr. B. Rech*

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Th. Frederking

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- Communication (Dr. I. Helms) GF-KOM
- Legal Matters and Contracts (Dr. U. Behrns) GF-RV
- Compliance Management (C. Pursian) GF-CM

Renewable Energy
Speaker: Prof. Dr. R. Schlatmann

- Silicon Photovoltaics (Prof. Dr. B. Rech) EE-IS
- Solar Fuels (Prof. Dr. R. van de Krol) EE-IF
- Competence Centre Photovoltaics Berlin (Prof. Dr. R. Schlatmann) EE-IP
- Nanoscale Structures and Microscopic Analysis (Dr. M. Wollgarten*) EE-ANSMA
- Interface Design (Prof. Dr. M. Bär) EE-NI
- Nano-SIPPE (Prof. Dr. C. Becker) EE-NSIP
- Operando Characterization of Solar Fuel Materials (Prof. Dr. K. Aziz-Lange) EE-NOC
- Perovskite Tandem Solar Cells (Dr. S. Albrecht) EE-NPET
- Operando Interfacial Photochemistry (Dr. R. Seidel) EE-NOGP
- Active Materials and Interfaces for Stable Perovskite Solar Cells (Dr. A. Abate) EE-NMIP
- Hybrid Materials Formation an Scaling (Dr. E. Unger) EE-NYFS
- Electrochemical Conversion of CO2 (Dr. M. Mayer) EE-NECC
- Molecular Systems (Prof. Dr. N. Koch) EE-GMS

Energy Materials
Speaker: Prof. Dr. S. Schorr

- Soft Matter and Functional Materials (Prof. Dr. M. Ballauff) EM-ISFM
- Applied Materials (Prof. Dr. J. Banhart) EM-IAM
- Institute for Nanospectroscopy (Prof. Dr. S. Raoux) EM-ISPEK
- Methods for Material Development (Dr. I. Wilkinson*) EM-IMM
- Functional Oxides for Energy Efficient Information Technologies (Dr. C. Dubourdieu) EM-IFOX
- Quantum Phenomena in Novel Materials (Prof. Dr. B. Lake) EM-IQM
- Structure and Dynamics of Energy Materials (Prof. Dr. S. Schorr) EM-ASD
- Methods for Characterization of Transport Phenomena in Energy Materials (Dr. habil. K. Habicht) EM-AMCT
- Materials for Green Spintronics (Prof. Dr. O. Rader) EM-AMGS
- Microstructure and residual stress analysis (Prof. Dr. Ch. Genzel) EM-AME
- Catalysis for Energy (Prof. R. Schlögl) EM-GKAT
- Berlin Joint Lab for Quantum Magnetism (Prof. Dr. J. Reuther) EM-NQUAM

Research with Large Scale Infrastructures
Speaker: Prof. Dr. A. Föhlisch

- Methods and Instrumentation for Synchrotron Radiation Research (Prof. Dr. A. Föhlisch) FG-ISRR
- Accelerator Physics (Prof. Dr. A. Jankowiak) FG-IA
- SRF – Science and Technology (Prof. Dr. J. Knobloch) FG-ISRF
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- Simulations of ERL-Design (Prof. A. Matveenko) FG-NSIMU
- Ultrafast Dynamics (Prof. Dr. M. Bargheer) FG-GUD

User Platform
Speaker: Prof. Dr. A. Jankowiak

- User Coordination (Dr. A. Vollmer) NP-ACO
- Operation Reactor BER II (S. Welzel) NP-ABR
- Operation Accelerator BESSY II (Prof. Dr. A. Jankowiak) NP-ABS
  - MLS Operation (K. Bürkmann-Gehrlein) S-MLS
- Protons for Therapie (Dr. A. Denker) S-PT
- Precision Gratings (Prof. Dr. M. Lörgen) S-PG
- High Field Magnet (Prof. Dr. B. Lake) NP-AHFM
- Optics and Beamlines (Dr. J. Viefhaus) NP-AOS
- Scientific-Technical Infrastructure 1 (Dr. A. Rupp) NP-HI
  - Technical User Support BER II (Dr. A. Rupp) NP-AUN
  - Sample Environments (Dr. K. Kiefer) NP-ASE
  - Procedural Management Decomissioning BER II (Dr. A. Rupp) NP-APMD
- Scientific-Technical Infrastructure 2 (Dr. C. Jung) NP-HII
  - Technical User Support BESSY II (R. Schulz) NP-AUP
  - Technical Design (L. Drescher) NP-ATD
  - Manufacturing (K. Tietz) NP-AMAN
- Macromolecular Crystallography (Prof. Dr. M. Wahl) NP-GMX
- X-Ray Microscopy (Prof. Dr. H. Ewers) NP-GXM

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- Experiment Control and Data Acquisition (O.-P. Sauer) IT-ED
- Infrastructure (Dr. D. Herrendörfer) IT-IS
- Representatives for Safety and Radiation Service (Th. Frederking)

Joint Laboratories

- Berlin Joint EPR Lab (BeJEL)
- Bielefeld-Berlin Joint Lab (BiBer)
- Joint Macromolecular Crystallography Laboratory (Joint MX Lab)
- Uppsala-Berlin Joint Lab (UBjL)
- Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE)
- Joint Ultrafast Dynamics Lab in Solutions and at Interfaces (JULiq)
- Joint Lab for Structural Research (JLSR)
- Joint Lab on Accelerator Physics (JLAP)

Projects

- Berlin Energy Recovery Linac Prototype (bERLinPro) (Prof. Dr. A. Jankowiak *Prof. Dr. J. Knobloch*)
- BESSY-VSR (Prof. Dr. A. Jankowiak Prof. Dr. J. Knobloch Prof. Dr. A. Föhlisch)
- Helmholtz Energy Materials Characterisation Platform (HEMCP) (Prof. Dr. R. Schlatmann)
- Dismantling of BER II (Dr. S. Welzel / *Dr. A Rupp*)
- Helmholtz Energy Materials Foundry (HEMF) (Prof. Dr. R. van de Krol)

Institute | Young Investigator Group Joint Laboratory | Joint Research Group | Working Group | Special Task | Committee

* Acting Head

Site map
The Lise-Meitner Campus with the research neutron source BER II is located at the HZB Berlin-Wannsee site, whereas the Wilhelm-Conrad-Röntgen Campus with the electron storage ring BESSY II is located at the HZB Berlin-Adlershof site.

IMPRINT

HZB Highlight Report 2016 of the Helmholtz-Zentrum Berlin für Materialien und Energie GmbH. Reprint only with the express permission of the publisher.
Press date: July 2017

Publisher:
Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin,
Tel.: +49 (0)30 80 62-420 34

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Publishing services & support:
n.k mediaconcept GbR, Obere Lagerstraße 38b,
82178 Puchheim bei München, Tel.: +49 (0)89 80 90 83 33
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Picture editing: Lothar Trutter

Proofs: Trumedia Gmbh, Tattenbachstraße 19, 86179 Augsburg

Print:
Elbe Druckerei Wittenberg GmbH, Breitscheidstraße 17a,
06886 Lutherstadt Wittenberg
Tel.: 03491 41 02 42, Fax: 03491 41 02 40
E-mail: info@elbedruckerei.de, www.elbedruckerei.de

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