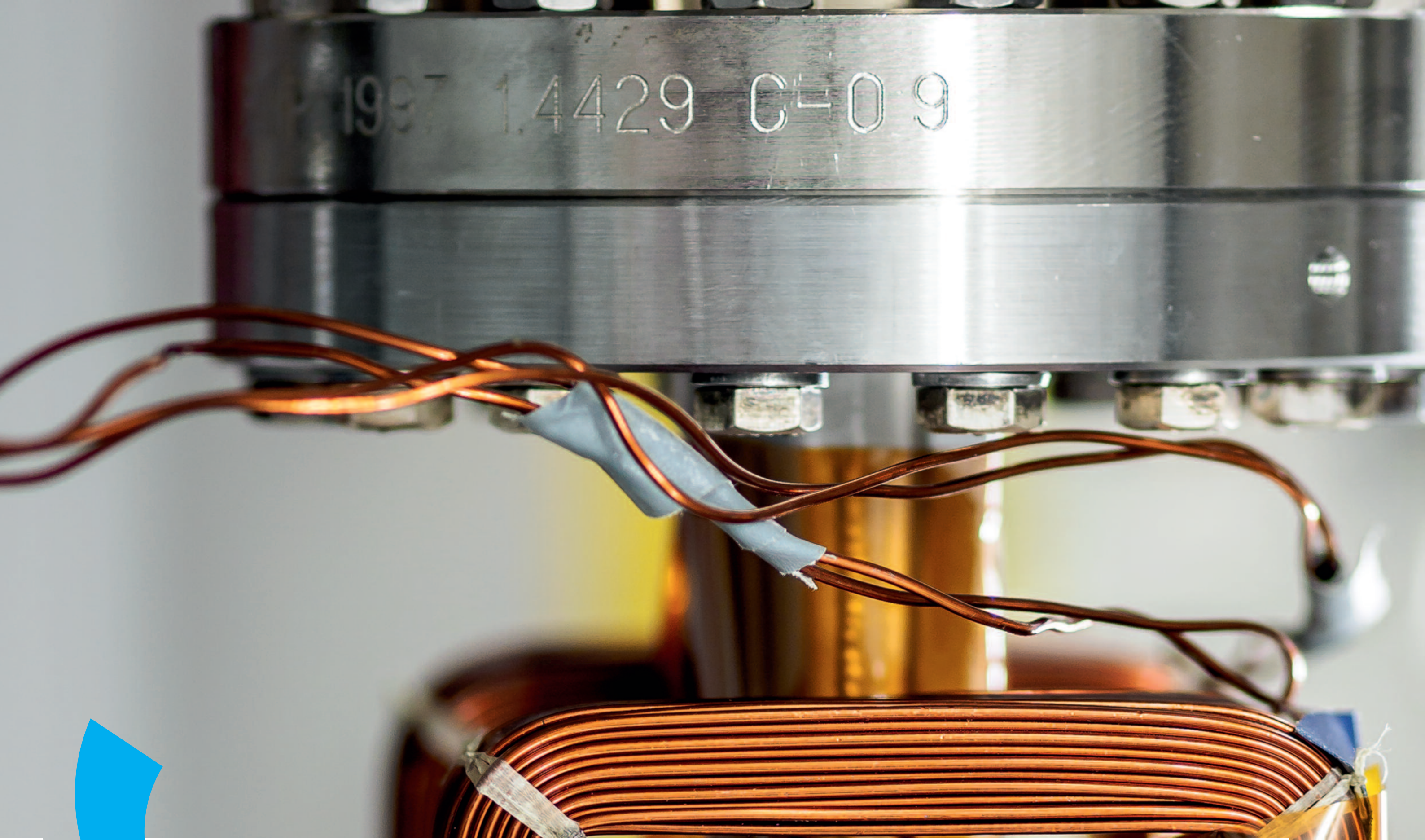
HZB Helmholtz Zentrum Berlin

FOCUSSING ENERGY REALISING VISIONS

HIGHLIGHTS 2017

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



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GREAT SUPPORT FOR BESSY III

In 2017 at HZB, the scientists themselves spent the entire year figuratively under a microscope – as their research was evaluated for the programme-oriented funding (POF). The review was concluded at the beginning of 2018 and the results are excellent. Once BESSY II has been upgraded into a variable-pulse-length storage ring, HZB will offer worldwide unique conditions for researching energy materials. The reviewers have also explicitly recommended that HZB start with the planning for BESSY III. While we so eagerly look to the future, we would also like to show you the excellent research results that were once again achieved at HZB in 2017.

Prof. Dr. Bernd Rech and Thomas Frederking.

One thing can be said that is true for both the regular reviews, by international experts, of HZB's organisational and scientific work and the experiments at HZB's large-scale facilities: the more thorough the preparation, the better the results. This is clearly reflected in the outstanding assessment of HZB's entire team following two on-site inspections in April 2018. The right decisions have been made, the review states, in the development of infrastructure and in the selection of personnel. All of HZB's research programmes have also been rated as excellent.

The fact that so many groups and programmes have received the highest marks of "Excellent" and "Outstanding" shows that HZB has chosen the right topics to work on, and is a top place for global energy and materials research. In order to maintain this position in the future, the reviewers have urged HZB to go ahead with the construction of BESSY III as the successor to the light source BESSY II. The upgrade programme BESSY VSR represents an important development along the route towards BESSY III and is explicitly commended and supported by the reviewers.

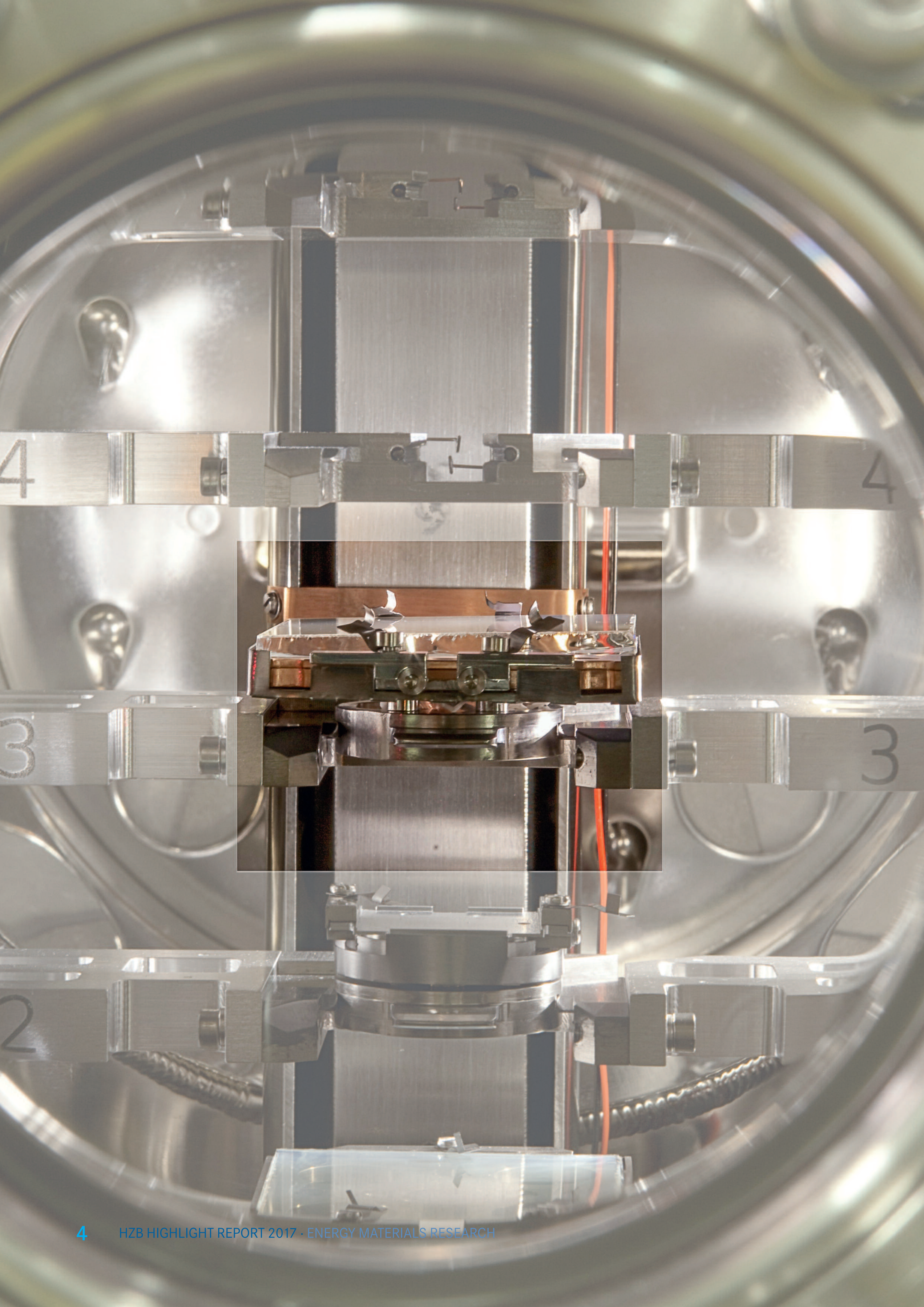
The review furthermore praises the excellent scientific results that HZB is already delivering in emerging and fast-growing research fields such as topological insulators and other exotic quantum materials. You can read up on research into quantum effects in solids, for example, on pages 10 to 12 in this report. Our researchers are also leaders in the field of perovskites for novel solar cells – more about that on page 8.

Currently, over 2,000 guest researchers come every year to make use of the experimental capabilities of the beamlines and instruments at the light source BESSY II and the research reactor BER II, some of which are unique in the world. We present a number of highlights from this research starting on page 20, such as new improvements in organic semiconductors and the examination of an ancient scavenger beetle fossilised in amber.

With that little teaser, dear readers, we wish you an informative read through our HZB Highlight Report 2017.

Prof. Dr. Bernd Rech
Scientific Director

Thomas Frederking
Administrative Director



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ENERGY MATERIALS RESEARCH

News in brief from HZB

On the 23rd of March 2017, the foundation stone was laid for a new laboratory building on the research campus in Wannsee that will be part of the **Helmholtz Energy Materials Foundry**. The building is now complete, offering ample space for a multitude of methods for synthesising and characterising energy materials. Among other things, it will be where materials are developed for converting carbon dioxide into hydrocarbons. The Institute for Functional Oxides for Energy Efficient Information Technologies (EM-IFOX), headed by Prof. Dr. Catherine Dubourdieu, will occupy the ground floor. Metal oxides such as those studied at EM-IFOX have an exceptionally broad spectrum of electric, magnetic, optical and mechanical properties, offering a huge potential for the development of new components.

Groups involved in the **Graduate School HyPerCells**, founded in 2015 by the University of Potsdam and HZB for research into perovskites, have produced perovskite solar cells with record efficiencies in excess of 20 per cent. Three Young Investigator Groups based at HZB have since joined HyPerCells. Currently, 15 doctoral students in the fields of chemistry, physics, electrical engineering and crystallography are researching here to deepen our understanding and to develop advanced materials and solar cell designs.

The **EU-sponsored research project INFINITE-CELL** in which HZB is participating began in November 2017. The goal of the project, which will run for four years, is to combine thin-film semiconductors made of silicon and kesterites into especially cost-effective tandem cells with efficiencies above 20 per cent. Several large research institutions from Europe, Morocco, the Republic of South Africa and Belarus will be working on the project, as will two partners from industry. Prof. Dr. Susan Schorr, head of the Structure and Dynamics of Energy Materials Department at HZB, will be contributing detailed experience with kesterite thin films and making the wide spectrum of analytical methods offered at HZB available for the project for very thorough characterisation of absorber materials.

HOW TO INCREASE EFFICIENCIES OF ULTRATHIN CIGSE SOLAR CELLS

Collaboration between a research group from HZB and a team from the Netherlands has set a new record for short-circuit current density in **ultrathin CIGSe solar cells**.

Ultrathin CIGSe solar cells require much fewer rare earth elements and less energy to produce. Unfortunately, they are much less efficient, too. The Young Investigator team Nanooptix at HZB has revealed how to prevent absorption loss in ultrathin CIGSe cells. Together with a group led by Prof. Albert Polman of the Institute for Atomic and Molecular Physics, Netherlands, they designed nanostructured back contacts featuring a silica nanopattern on ITO for trapping light in ultrathin CIGSe cells. Combined with a back reflector and an anti-reflection layer, the record-breaking cell has a short-circuit current density of 34 mA/cm^2, which is the highest value in any ultrathin CIGSe cell to date, reaching 93 per cent of the short-circuit current density of the standing champion thick cells.
More intriguingly, the nanostructured back contacts also improve the cells' electrical performance, yielding an efficiency enhancement of 47 per cent relative to flat cells of equal thickness. "The achievements prove that the nanostructures are able to simultaneously benefit ultrathin CIGSe solar cells from both optical and electrical aspects", claims Guanchao Yin, first author of the publication. "This result shows that optoelectronic nanopatterning provides a path to high-efficiency cells with reduced material consumption", adds Prof. Martina Schmid, who has joined University of Duisburg as a professor for experimental physics.

arö

Nanostructures trap the light, as this illustration on the cover of Advanced Optical Materials shows.

Advanced Optical Materials, 5, 2017 (DOI: 10.1002/adom.20160637): Optoelectronic Enhancement of Ultrathin CuIn1–xGaxSe2 Solar Cells by Nanophotonic Contacts; G. Yin et. al.

REVEALING DEFECTS IN KESTERITE SEMICONDUCTORS WITH NEUTRONS

A research team at HZB has for the first time precisely characterised the various types of defects in kesterite semiconductors. The findings point to a means of guided optimisation for kesterite solar cells.

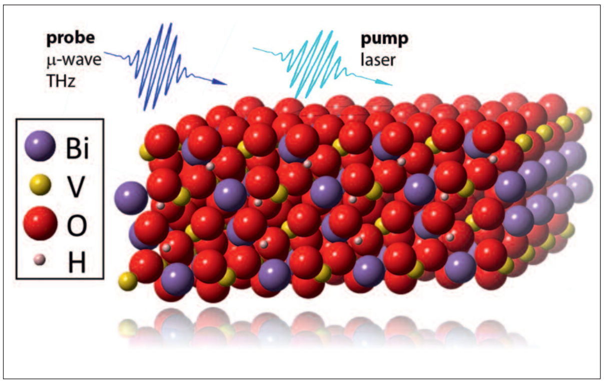
Kesterites consist of copper, zinc, tin and selenium and are semiconducting and able to convert light into electricity. The highest efficiency levels are achieved with CZTSe absorber layers that contain somewhat less copper in comparison to the standard chemical formula and somewhat more zinc. This kind of stoichiometric deviation leads to defect sites in the crystal structure that, oddly, seem to increase the level of efficiency. "We have now precisely characterised these defect sites and ascertained their local concentrations with the help of neutron diffraction experiments", explains Dr. Galina Gurieva from the HZB Structure and Dynamics of Energy Materials group. The method is ideal for this characterisation, as copper and zinc can be differentiated from each other extremely well using neutrons. The team investigated 29 different CZTSe powder samples, some of them at BER II. They were able to identify sites in the crystal structure where a copper atom was missing or where they were occupied by an element other than the anticipated element. So-called copper/zinc disorder plays an important role as well: copper atoms are sitting on zinc sites in the crystal structure and vice versa. "The point defects we investigated experimentally really correspond quite well to the theoretical model of potential defects", declares Gurieva: "We can deduce concrete clues from this study as to which point defects in which concentration to expect in the given composition of kesterite thin films. This may help to optimise kesterite-based solar cells further." *arö*

JAP 123, 161519 (DOI: 10.1063/1.4997402): Intrinsic point defects in off-stoichiometric $Cu_2ZnSnSe_4$: A neutron diffraction study; G. Gurieva et. al.

CHARGE CARRIERS WITH A LONG LIFE SPAN

At HZB, a team of scientists analysed how a special treatment improves **metal-oxide photoelectrodes**. Their results are paving the way to more efficient and cheaper devices for solar hydrogen production.

Basically, our energy supply relies heavily on fossil resources. But the fossil fuel age is bound to end for several strong reasons. As an alternative to fossil fuels, hydrogen seems very attractive. The gas has a huge energy density, it can be stored or processed further, e.g. into methane, or it can directly provide clean electricity via a fuel cell. If produced using sunlight alone, hydrogen is completely renewable with zero carbon emissions.
Similar to a process in natural photosynthesis, sunlight can also be used in "artificial leaves" to split water into oxygen and hydrogen. Artificial leaves combine photoactive semiconducting materials and can reach efficiencies beyond 15 per cent. That is considerably higher than their natural counterparts, whose efficiencies are no higher than one or two per cent. However, those record efficiencies were obtained using expensive systems, which also tend to decompose in aqueous solutions. For successful commercialisation, costs need to decrease and stability needs to increase.



Using time-resolved conductivity measurements in hydrogen-treated bismuth vanadate ($BiVO_4$), researchers have shown that electrons and holes last twice as long in this material. This increases the material's efficiency as a photoelectrode.

Good candidates, with one disadvantage

Complex metal-oxide semiconductors are good candidates for artificial leaves since they are relatively cheap and stable in aqueous solutions. Scientists from the HZB Institute for Solar Fuels are focusing their research on these materials. Until now, photoelectrodes based on metal oxides have exhibited only moderate efficiencies of less than eight per cent. One reason is their poor charge-carrier (electron/hole) mobility, which can be as much as 100,000 times lower than in classi semiconductors such as gallium arsenide or silicon. "What is worse is the fact that charge carriers in metal oxides often have really short life spans of nanoseconds or even picoseconds. Many of them disappear before they can contribute to water splitting", Dr. Fatwa Abdi, expert at HZB-Institute for Solar Fuels, points out.
One option to overcome this limitation is heat treatment under a hydrogen atmosphere of the metal oxide layers after deposition. Fatwa Abdi and his colleagues have now investigated how this treatment influences life spans, transport properties and defects in one of the most promising metal-oxide photoelectrodes, bismuth vanadate ($BiVO_4$).

Life spans of charge carriers doubled

Time-resolved conductivity measurements revealed that electrons and holes live more than twice as long in the bulk of the hydrogen-treated $BiVO_4$ as in pristine $BiVO_4$. As a result, the overall photocurrent under sunlight is largely improved. Further measurements in Dresden and theoretical calculations by KAUST colleagues in Saudi Arabia have provided evidence that the presence of hydrogen in the metal oxide reduces or deactivates point defects in the bulk of $BiVO_4$. "Our results show that hydrogen treatment leads to fewer traps for charge carriers and fewer opportunities to recombine or become lost. So, more charge carriers survive for longer and may contribute to water splitting", Abdi explains.

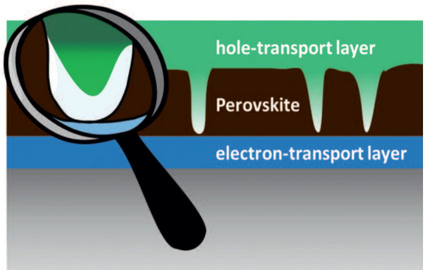
arö

Advanced Energy Materials, 2017 (DOI: 10.1002/aenm. 201701536): Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment; J.-W. Jang, D. Friedrich, S. Müller, M. Lamers, H. Hempel, S. Lardhi, Z. Cao, M. Harb, L. Cavallo, R. Heller, R. Eichberger, R. van de Krol and F. F. Abdi

PERFECTION IS NOT REQUIRED IN PEROVSKITE SOLAR CELLS

A team from HZB working at BESSY II has discovered why **thin perovskite layers** achieve amazingly high efficiencies despite their many holes.

Thin films made of low-cost metal-organic perovskites can be produced on a large scale, for example, by spin coating on a substrate and subsequent baking. However, the thin perovskite films that result from this procedure are generally not perfect, and instead exhibit many holes. Logically these holes ought to create short-circuits in the solar cell and thus reduce the level of efficiency considerably. Prof. Marcus Bär and his group, together with the Spectro-Microscopy group of the Fritz Haber Institute, have carefully examined samples from the pioneering group led by Prof. Henry Snaith of the University of London. Using scanning electron microscopy, they mapped the surface morphology. They subsequently analysed the chemical composition of the samples in those areas exhibiting holes using spectromicrographic methods at BESSY II. "We were able to show that the substrate was not really exposed even in the holes, but instead a thin layer builds up essentially as a result of the deposition and crystallisation processes there, which apparently prevent short-circuits", explains doctoral student Claudia Hartmann.
The scientists ascertained at the same time that even in the event of a direct encounter of the contact layers, the charge carriers have to overcome a relatively high energy barrier if they are to recombine with one another. "The electron transport layer (TiO_2) and the transport material for positive charge carriers (Spiro MeOTAD) do not actually come into direct contact. In addition, the recombination barrier between the contact layers is sufficiently high that the losses in these solar cells is minute, despite the many holes in the perovskite thin-film", says Bär. *arö*



Simplified cross-section of a perovskite solar cell: the perovskite layer does not cover the entire surface, but instead exhibits pinholes. The scientists showed that a protective layer builds up, preventing short-circuits.

Advanced Materials Interfaces, 2018 (DOI: 10.1002/admi.201701420): Spatially Resolved Insight into the Chemical and Electronic Structure of Solution–Processed Perovskites – Why to (Not) Worry about Pinholes; C. Hartmann et. al.

MESOPOROUS INTERFACE MITIGATES THE IMPACT OF DEFECTS

Two teams, from HZB and TU München, have revealed the influence of internal architecture on the stability of perovskite solar cell efficiency.

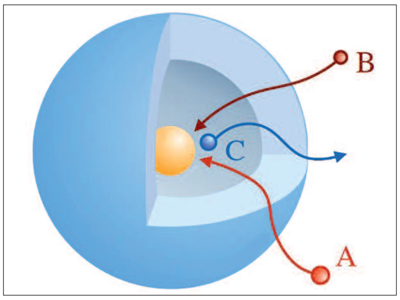
The conversion efficiencies of perovskite thin films decrease sharply when the material is exposed to UV radiation and electric fields, as is the case in real operating conditions. Dr. Antonio Abate, head of a Helmholtz Young Investigators Group at HZB, and Prof. Allessio Gagliardi, TU Munich, therefore explored two different types of architecture of perovskite solar cells: one group of cells had a planar interface between the perovskite and a metal-oxide electron transport layer, while the other was built up as a mesoporous interface of intermingling perovskite and metal oxide to form a complex sponge-like structure. After careful experimental observations and numerical simulations, the scientists not only proved that the perovskite cell with the mesoporous interface exhibits better output stability over time, but were also able to provide an explanation as to why: "The benefit induced by the mesoporous interface is fundamentally due to its large surface area", Abate explains. Defects that compromise the power output and operating life which accumulate in the electron transport layer during operation tend to get diluted in this large surface. *arö*

ACS Energy Letters, 2018, 3 (1), pp 163–169 (DOI: 10.1021/acsenergylett.7b01101): Mesoporous Electron-Selective Contacts Enhance the Tolerance to Interfacial Ion Accumulation in Perovskite Solar Cells, A. Gagliardi and A. Abate

A MODEL FOR A WIDE RANGE OF RESEARCH FIELDS

A theoretical team from HZB has mathematically described how two different molecules react with each other **in nanoreactors**. This allows predictions of how reactions can be better controlled.

Nanoreactors are tiny systems that facilitate specific chemical reactions. Many are found in biological systems, but chemists are also able to synthesise artificial nanoreactors to control chemical reactions. An important class of these has a "yolk-and-shell" architecture like an egg: a catalytically active metallic nanoparticle is surrounded by a shell consisting of a polymeric network. These kinds of nanoreactors can create isolated environments for specific reactions. "We have now mathematically described for the first time how two different molecules are transported to react within nanoreactors. The new model shows clearly what factors favour a given reaction", says Dr. Rafael Roa, first author of the publication. Roa is a postdoc in the group led by Prof. Joe Dzubiella at the HZB Institute for Soft Matter and Functional Materials.
Some of the results come as a surprise: contrary to expectations, the reaction rate is limited not so much by the concentration of molecules in solution, but decisively by the permeability of the nanoreactor's shell. "This is extremely interesting since chemists today can often fine-tune or even switch the permeability of these shells to specific molecules via variations in temperature or other parameters", explains co-author Dr. Won Kyu Kim. Dzubiella's Soft Matter Theory group collaborates with HZB chemist Prof. Yan Lu, an acknowledged expert in synthetic nanoreactors. They are eager to test their theoretical predictions on real systems. *arö*



Sketch of a yolk-and-shell-type nanoreactor: reactands A and B diffuse through the shell and react to form C at the catalytically active nanoparticle (yellow).

ACS Catal., 2017, 7 (9), 5604–5611 (DOI: 10.1021/acscatal.7b01701): Catalyzed Bimolecular Reactions in Responsive Nanoreactors; R. Roa, W. Kyu Kim, M. Kanduč, J. Dzubiella and S. Angioletti-Uberti

BETTER CATHODE MATERIALS FOR LITHIUM-SULPHUR BATTERIES

Scientists at HZB have for the first time fabricated a nanomaterial made of a titanium oxide compound with an extremely large surface area. This highly porous material possesses a high and constant storage capacity.

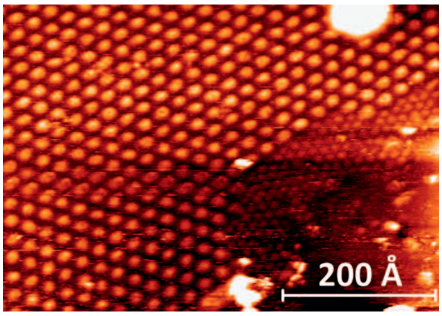
Lithium-sulphur batteries are considered to be a low-cost and environmentally friendly alternative to lithium batteries. As lithium ions migrate to the cathode during the discharge cycle, a reaction takes place at the cathode that forms lithium sulphide (Li_2S) as well as lithium polysulphides, which cause the battery's capacity to decline over the course of multiple charging cycles. For this reason, research teams are working to improve cathode materials that would be able to encapsulate polysulphides, for example, with nanoparticles made of titanium dioxide (TiO_2). The HZB team headed by Prof. Yan Lu has now fabricated a cathode material where nanoparticles of Ti_4O_7 molecules provide confinement of the sulphur. X-ray spectroscopy measurements (XPS) at the CISSY experiment of BESSY II show that sulphur compounds bind strongly to the surface in the nanomatrix. This also accounts for the high specific capacity that declines very little during repeated charge cycles (0.094 per cent per cycle). "We have been working to improve the repeatability of this synthesis for over a year. Next, we will work on fabricating the material as a thin-film", says Yan Lu. Then, the whole process can be transferred to commercial manufacturing because all of its steps are scalable. *arö*

Advanced Functional Materials, 2017 (DOI: 10.1002/adfm.201701176): Porous Ti_4O_7 Particles with Interconnected-Pores Structure as High-Efficiency Polysulfide Mediator for Lithium-Sulfur Batteries; S. Mei, C. J. Jafta, I. Lauermann, Q. Ran, M. Kärgell, M. Ballauff and Y. Lu

A SOFA STRUCTURE FOR THE CONTROL OF SPINS

Gold-doped graphene is hailed as a material for future information technologies because its spins can be controlled. Researchers at HZB have now discovered exactly how this works.

Graphene is probably the most exotic form of carbon: all of the atoms are bound to one another solely in a monolayer, forming a matrix of hexagons like a honeycomb. Graphene is extremely thin, conductive, transparent and quite strong. Its structure also makes it possible to control the spins (tiny magnetic moments) of the conduction



Scanning Tunnelling Microscopy shows the regular corrugation pattern of graphene over clusters of gold.

electrons extremely well. Surprisingly, if you apply a layer of graphene to a nickel substrate and shove atoms of gold in between, then what is known as the spin-orbit interaction dramatically increases by a factor of 10,000, allowing the orientation of the spins to be influenced by external fields.

Physicists working with Dr. Andrei Varykhalov at HZB had already demonstrated several times that this works. “We wanted to discover how it happens that the high spin-orbit interaction, which is characteristic of gold, is transferred over to graphene”, says Varykhalov. The physicists discovered that the atoms of gold are not distributed completely uniformly in the interlayer, but instead huddle together on the nickel substrate in small groups or clusters. These gold clusters in turn form a regular pattern beneath the graphene. Between these clusters, nickel atoms remain uncovered by gold. Graphene binds strongly to the exposed nickel, arching over the gold clusters. “It looks almost like a bolster of material on a chesterfield sofa”, explains Varykhalov. “At the points where the gold and carbon come into close contact, we observed an extremely strong spin-orbit interaction. This result was supported by scanning tunnelling microscopy and analyses using density functional theory.” *arö*

2D Materials, Vol. 4, Nr. 3, 2017 (DOI: 10.1088/2053-1583/aa7ad8): Nanostructural origin of giant Rashba effect in intercalated graphene; M. Krivenkov et. al.

THE MISSING LINK BETWEEN NEW TOPOLOGICAL PHASES OF MATTER HAS BEEN FOUND

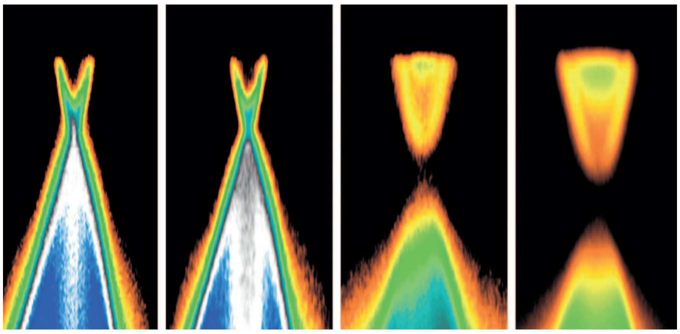
HZB physicists at BESSY II have discovered a **ferroelectric phase** within a topological insulator that can be reversed by an external electric field. This could lead to new applications such as switching between different conductivities.

The HZB researchers studied crystalline semiconductor films made of a lead, tin and selenium alloy (PbSnSe) that were additionally doped with tiny amounts of the element bismuth. These semiconductors belong to the new class of materials called topological insulators, materials that conduct very well at their surfaces while behaving as insulators internally. Now, doping with 1–2 per cent bismuth has enabled them to observe a new topological phase transition. The sample enters a particular topological phase that also possesses the property of ferroelectricity. This means that an external electric field distorts the crystal lattice while, conversely, mechanical forces on the

lattice can create electric fields. This effect can be used to develop new functionalities, which is also of interest for potential applications. Ferroelectric phase-change materials are employed in DVDs and flash memories, for example. An electric voltage displaces atoms in the crystal, transforming the insulating material into a metallic one. The investigation was conducted in close collaboration with researchers from Johannes-Kepler-Universität Linz, who also grew the samples. Partha S. Mandal, who carried out the measurements on the material system as part of his dissertation, was supported by the Helmholtz Virtual Institute "New States of Matter and their Excitations".
The bismuth doping of PbSnSe films investigated at HZB created perturbations. The number of electrons in bismuth does not fit well in the periodic arrangement of atoms within the PbSnSe crystal. "Tiny changes in the atomic structure give rise to fascinating effects in this class of materials", explains HZB researcher Dr. Jaime Sánchez-Barriga, principal investigator coordinating the project.

Ferroelectric distortion in the crystal lattice

Following detailed analyses of the measurements, only one conclusion remained: the bismuth doping causes a ferroelectric distortion in the lattice that also changes the allowable energy levels of the electrons. "This problem kept us puzzled during several beamtimes until we reproduced the scientific results on a whole new set of samples", adds Sánchez-Barriga. "Potential applications could arise through ferroelectric phases – ones that have not been thought of before. Lossless conduction of electricity in topological materials can be switched on and off at will, by electrical pulses or by mechanical strain", explains Prof. Oliver Rader, head of the department Materials for Green Spintronics at HZB. *arö*



Bismuth doping is enhanced from 0 per cent (left) to 2.2 per cent (right). Measurements at BESSY II show that this leads to larger bandgaps.

Nature Communications, Vol. 8, Art. 968 (DOI: 10.1038/s41467-017-01204-0): Topological quantum phase transition from mirror to time reversal symmetry protected topological insulator; P. S. Mandal et. al.

NEW SWITCHING PROCESS IN SPINTRONICS DEVICES

A team of several German institutes achieved a robust and reliable magnetisation switching process by domain wall displacement without any applied fields. The effect is observed in tiny asymmetric permalloy rings, and may pave the way to extremely efficient new memory devices.

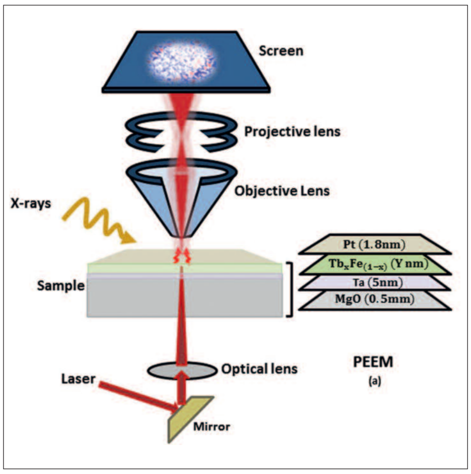
To construct magnetic memories, elements with two stable magnetisation states are needed which can be switched in both directions. Promising candidates for such magnetic elements are tiny rings, typically on the order of few micrometres, with clockwise or anticlockwise magnetisation as the two states. Unfortunately, directly switching between those two states requires a circular magnetic field, which is not easy to achieve. But this problem can be solved, as demonstrated by a team of scientists from several institutions in Germany: if the hole in the ring is slightly displaced, thus making the ring thinner on one side, a simple, uniaxial magnetic field pulse of some nanoseconds in duration is sufficient to switch the magnetisation between the two possible "vortex states", clockwise and anticlockwise.
The scientists recorded the time evolution of the magnetisation dynamics of the device at the Maxymus-Beamline at BESSY II employing time-resolved x-ray microscopy during and after the short magnetic field pulse was applied. They observed how the magnetic field pulse leads in a first step to an intermediate "onion state" in the ring. This state is characterised by two domain walls, where different magnetisation zones meet each other. After the external field pulse has vanished, these domain walls move towards each other and annihilate, which results in a stable opposite magnetisation of the ring's "vortex state". "Our measurements show domain wall automotion with an average velocity of about 60 m/s. This is very fast for spintronic devices at zero applied field", lead author of the publication Dr. Mohamad-Assaad Mawass points out. "We believe to have identified a robust and reliable switching process by domain wall automotion in ferromagnetic rings", Mawass states. "This could pave the way for further optimisation of these devices." *arö*

Phys. Rev. Applied 7, 044009 (DOI: 10.1103/PhysRevApplied.7.044009): Switching by Domain-Wall Automotion in Asymmetric Ferromagnetic Rings; M.-A. Mawass, K. Richter, A. Bisig, R. M. Reeve, B. Krüger, M. Weigand, H. Stoll, A. Krone, F. Kronast, G. Schütz, and M. Kläui

OPTICAL CONTROL OF MAGNETIC MEMORY

A research team at HZB has shown how **laser modulation of magnetic properties in materials** can be influenced. The results give important clues for the theoretical understanding of optically controlled magnetic data storage media.

Rapidly increasing quantities of data and new technological applications are demanding memory that can store large amounts of information in very little space and permit this information to be utilised dependably at high access speeds. Rewriteable magnetic data storage devices using laser light appear to have especially good prospects. Researchers have been working on this new technology for several years. “However, there are still unresolved questions about the fundamental mechanisms and the exact manner in which optically controlled magnetic storage devices operate”, says Dr. Florian Kronast, assistant head of the Materials for Green Spintronics Department at HZB.



Schematic of the experiment set-up.

A research team led by Kronast empirically established that the warming of the storage material by the energy of the laser light plays an instrumental role when toggling the magnetisation alignments, and that the change in the material only takes place under certain conditions.

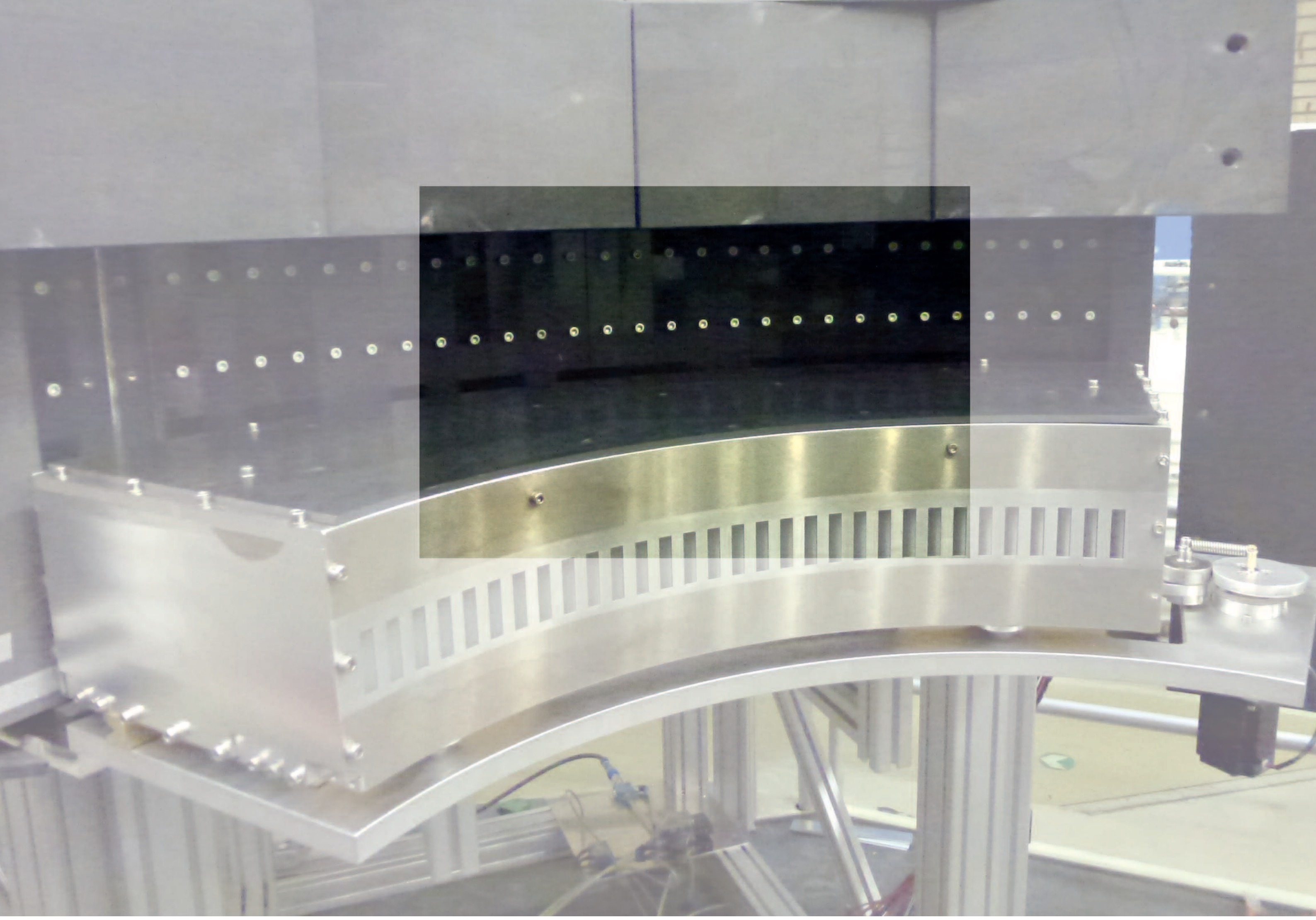
Making precise measurements in tiny laser spots

The HZB scientists together with those of Freie Universität Berlin and Universität Regensburg irradiated a thin layer of magnetic material using circularly polarised laser light and studied the microscopic processes at extremely high resolution. To do this, they directed the light of an infrared laser onto a nanometre-thick layer of alloy made from the metals terbium and iron (TbFe). What was special about the experimental set-up was that the narrowly focused spot of laser light had a diameter of only three microns. “That is far less than was usual in prior experiments”, says HZB scientist Ashima Arora, first author of the study. And it provided the researchers with a resolution of unsurpassed detail for studying the phenomena. The images of the magnetic domains in the alloy, which the team created with the help of X-rays from the BESSY II synchrotron radiation source, revealed fine features a mere 30 nanometres in size.

The results of the measurements prove that a ring-shaped region forms around the tiny laser spot and separates the two magnetically contrasting domains from one another. The extant magnetisation pattern inside the ring is completely erased by the thermal energy of the laser light. Outside the ring, however, it remains in its original state. Within the boundary zone itself, a temperature distribution arises that facilitates a change in magnetisation by displacing the domain boundaries. “It is only there that the toggling of magnetic properties can proceed, permitting a device to store rewriteable data”, explains Arora.

“These new insights will assist in the development of optically controlled magnetic storage devices having the best possible properties”, Kronast believes. An additional effect contributes to a better understanding of the physical processes that are important in this phenomenon, which researchers at HZB unexpectedly observed for the first time. The way the toggling of the magnetisations happens is highly dependent on the layer thickness of the material irradiated by the laser. It changes over an interval of 10 to 20 nanometres thickness. “This is a clear indication that two contrasting mechanisms are involved and compete with one another”, Kronast explains. He and his team suspect there are two complex physical effects behind this. To confirm their suspicions and find out which of the two effects is responsible, however, further studies are necessary. *rb/HZB*

Scientific Reports, Vol. 7, Art. 9456, 2017 (DOI: 10.1038/s41598-017-09615-1): Spatially resolved investigation of all optical magnetisation switching in TbFe alloys; A. Arora, M.-A.-Assaad Mawass, O. Sandig, C. Luo, A. A. Ünal, S. Radu, S. Valencia, and F. Kronast



DEVELOPING METHODS FOR RESEARCH AT HZB'S LARGE-SCALE FACILITIES

The triple-axis spectrometer FLEXX at BER II is a device for measuring magnetic excitations and lattice vibrations. There is typically a characteristic relationship between excitation energy and scattering angle. One data point at FLEXX measures exactly one angle and one energy transfer, where each measurement can take several seconds to several minutes, depending on the sample. Researchers are of course keen to measure as many angles and energies as quickly as possible.

The new detector module MultiFLEXX, developed by the FLEXX team and assembled in the HZB workshops, does exactly that. It measures 31 angles and 5 energy transfers simultaneously, being composed of 155 analysers and detectors. Each MultiFLEXX data point has a count rate 5 to 10 times shorter than a single data point at FLEXX – thus increasing acquisition efficiency by more than a factor of 10. This is especially interesting for users who want to map out an excitation as a function of temperature or magnetic field – frequent applications at FLEXX. The new detector module has already tested successful in several experiments, both by external users and in HZB's own research on thermoelectrics.

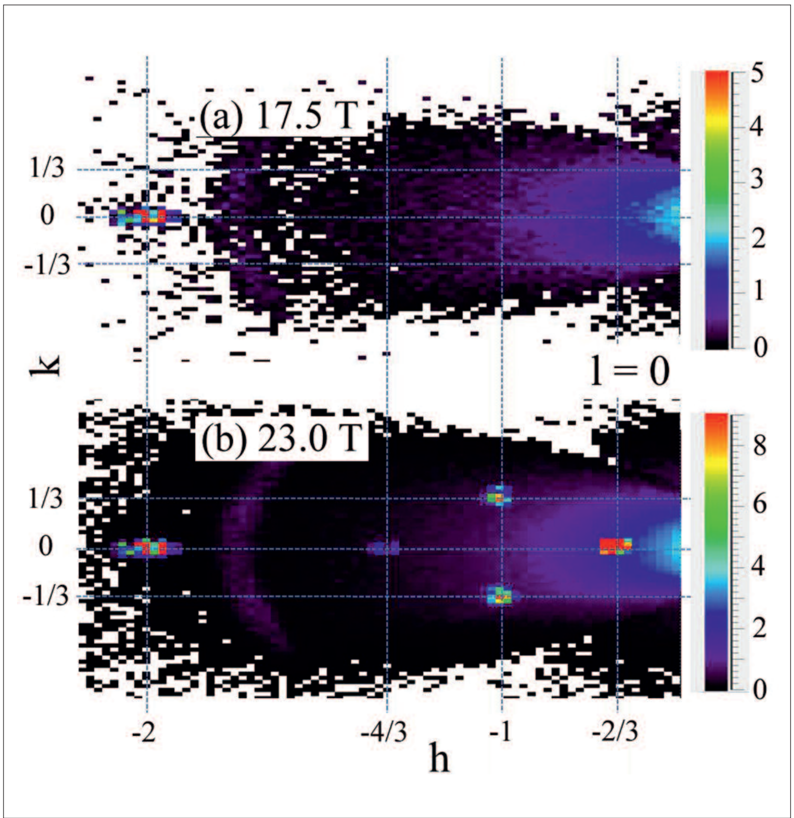
News in brief from HZB

HIGH-FIELD MAGNET AT BER II GIVES AN INSIGHT INTO A HIDDEN ORDER

For quite some time, researchers have been puzzled by how **a certain uranium compound changes** its crystalline structure at very cold temperatures. A team of physicists at HZB has managed to solve the puzzle using the High-Field Magnet at BER II, where neutron experiments can be performed under extremely high magnetic fields.

Crystals comprising the elements uranium, ruthenium, rhodium and silicon have a simple geometric structure, and ought to be holding no more secrets for scientists. However, that is not the case – quite the contrary. At temperatures below 17.5 kelvins, a new internal order emerges: something in the material changes in some as yet undiscovered way, releasing a certain amount of heat as a signature. Known is only that this order is not due to static magnetic moments. More than a thousand publications have already appeared on this topic without having lifted the veil.

However, conventional magnetic states can be induced in various ways such as by doping or by applying pressure or strong magnetic fields. This may help to shed more light on the hidden order itself. In order to at least study new magnetic states emerging from the hidden order, physicists from the HZB, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), the University of Amsterdam and Leiden University, Netherlands, have investigated flawless crystals made of $U(Ru_{0.92}Rh_{0.08})_2Si_2$ under cryotemperatures and extremely high magnetic fields using neutrons.



Additional spots appear on the neutron detector starting at a magnetic field strength of 23 teslas, revealing the new magnetic order in the crystal.

New magnetic order above 21.6 teslas

"The neutron scattering experiments conducted under extremely high magnetic fields have shown that at about 21.6 teslas, there really is a new magnetic phase transition", explains first author Dr. Karel Prokeš from HZB. "This means that a new magnetic order has become established in the crystal." This involves an uncompensated antiferromagnetic order in which the magnetic moments of the uranium atoms point in alteration up-up-down in opposite directions.

Incidentally: when Prokeš submitted the joint manuscript to the renowned journal Physical Review B, he received a positive reply within 19 minutes. The work was published as a "Rapid Communication" – a new speed record which says a lot about the importance of this experiment for solid-state physics.

arö

Phys. Rev. B 96, 121117(R), (DOI: 10.1103/PhysRevB.96.121117): Magnetic structure in a $U(Ru_{0.92}Rh_{0.08})_2Si_2$ single crystal studied by neutron diffraction in static magnetic fields up to 24 T;
K. Prokeš, M. Bartkowiak, O. Rivin, O. Prokhnenko, T. Förster, S. Gerischer, R. Wahle, Y.-K. Huang, and J. A. Mydosh

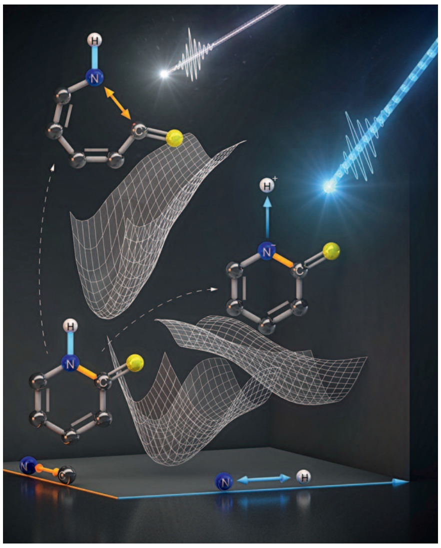
HOW DNA PROTECTS ITSELF AGAINST LIGHT

A team at HZB, together with researchers in Sweden and the USA, has observed how the energy of **incoming photons can be absorbed by biomolecules** without destroying important bonds. A very sensitive method available at BESSY II was used for the experiments.

When the molecules that carry the genetic code in our cells are exposed to harm, they have defences against potential breakage and mutations. For instance, when DNA is hit with ultraviolet light, it can expel excess energy from the radiation by ejecting the nucleus of a hydrogen atom – a single proton – to keep other chemical bonds in the system from breaking. To gain insight into this process, researchers used X-ray laser pulses from the Linac Coherent Light Source (LCLS) at the Department of Energy's SLAC National Accelerator Laboratory to investigate how energy from light transforms a relatively simple molecule called 2-thiopyridone. This molecule undergoes a chemical transformation that also occurs in the building blocks of DNA.
The investigation was done within Virtual Institute VI419, funded by the Helmholtz Association, which was established by HZB jointly with the University of Potsdam and the University of Stockholm, and involves a team at the University of Washington and at the SLAC National Accelerator Laboratory operated by Stanford University for the U.S. Department of Energy's Office of Science.

Enlightening comparison of experimental data

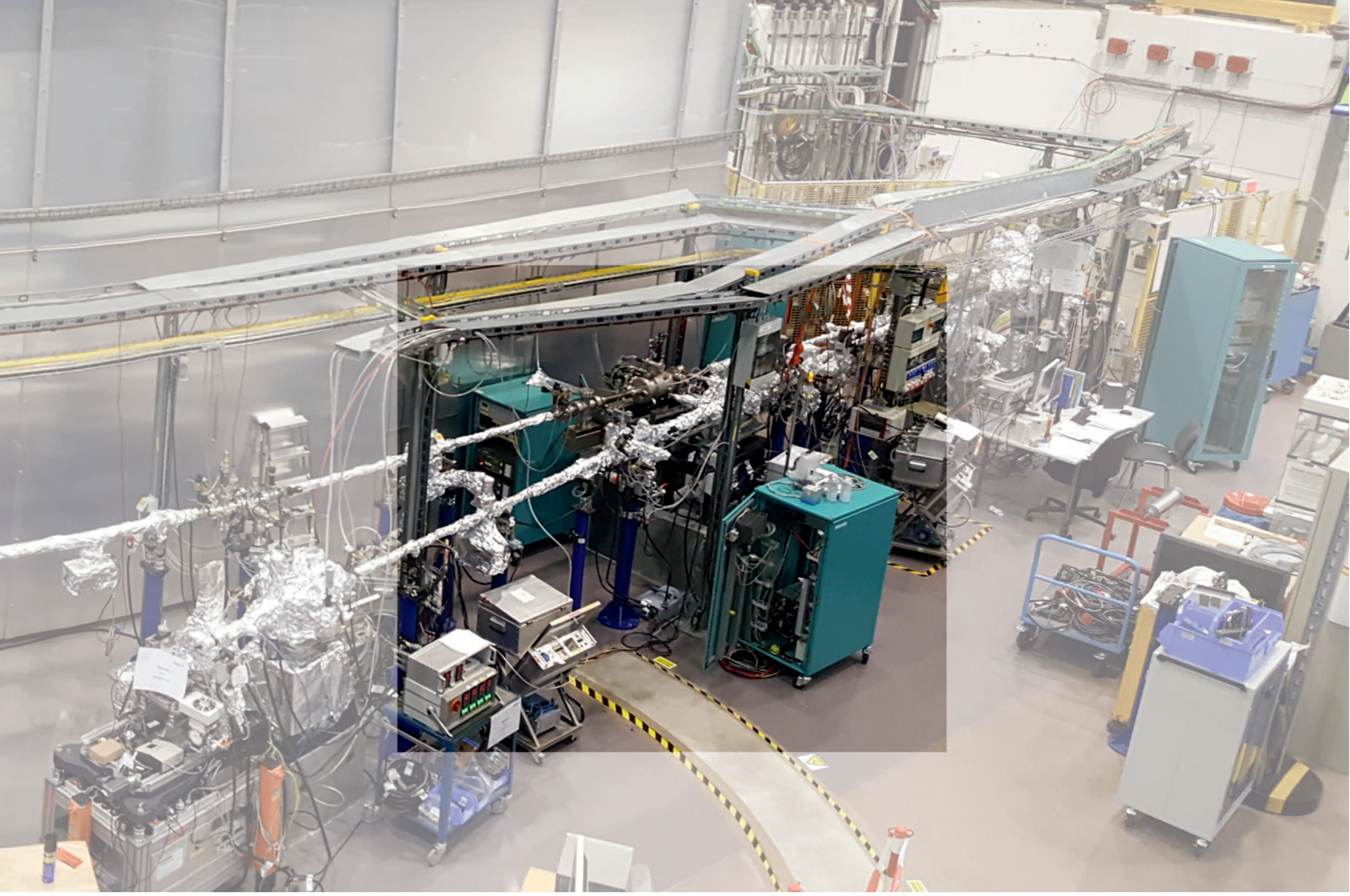
The scientists observed this process by probing the nitrogen atom in the molecule with X-ray pulses lasting mere femtoseconds, or quadrillionths of a second. The results show, in detail, how the proton bound to the nitrogen atom is ejected when excited by the light pulse. This is an important step towards a better understanding of what's called "excited-state proton transfers" in DNA and other molecules. "Right now, we want to keep it simple", says lead author Sebastian Eckert, who is completing his doctoral studies at the University of Potsdam and HZB, which are funded by an EDAX ERC Grant gained by Prof. Alexander Föhlisch. "It's easier to look at the effects of photoexcitation in 2-thiopyridone because this molecule is small enough to understand and has only one nitrogen atom. Only by comparing the FEL measurements with experiments at the synchrotron BESSY II could the mechanism be clearly understood." It was also the first time the method,



The experimental data show how a light pulse dissociates a hydrogen nucleus from the nitrogen atom without destroying important bonds within the molecule.

known as resonant inelastic X-ray scattering or RIXS, has been used at BESSY II to observe molecular changes involving nitrogen that occur in femtoseconds. This short timescale is important because that is how fast protons are kicked away from molecules exposed to light, and it requires brilliant X-rays to see these ultrafast changes.
By combining the experiments with theoretical simulations, the reaction pathway was ultimately elucidated. Doctoral student Jesper Norell and Prof. Dr. Michael Odelius of the University of Stockholm performed these calculations in the scope of the Helmholtz Virtual Institute "Dynamic Pathways in Multidimensional Landscapes". Next, the collaboration will use the same approach to study more complex molecules and gain insights into the wide class of photochemical reactions. *arö*

Angew. Chem. Int. Ed. 2017, Vol. 56, Issue 22, 6088-609 (DOI: 10.1002/anie.201700239): Ultrafast Independent N-H and N-C Bond Deformation Investigated with Resonant Inelastic X-ray Scattering; S. Eckert, J. Norell, P. S. Miedema, M. Beye, M. Fondell, W. Quevedo, B. Kennedy, M. Hantschmann, A. Pietzsch, B. Van Kuiken, M. Ross, M. P. Minitti, S. P. Moeller, W. F. Schlotter, M. Khalil, M. Odelius and A. Föhlisch



ACCELERATOR RESEARCH AND DEVELOPMENT

News in brief from HZB

The **X-ray microscope HZB-TXM** is back in operation. The TXM allows, for example, element-specific imaging of important molecular processes in cell membranes and in catalysis involving silicon, sulphur and phosphorus – now in far superior quality compared to the predecessor model. Images taken of identical test objects clearly demonstrate the benefits of the new TXM. The X-ray microscope is installed at the U41-L06-PGM1-XM beamline, which was newly set up in the summer of 2017 to deliver beams in the "tender X-ray" regime, namely in the energy range between 2 keV and 2.5 keV.

The beamline design was developed in cooperation with Rolf Follath (now at PSI, Switzerland). The set-up of the beamline itself was supported by the Institute for Nanometre Optics and Technology (mainly by Matthias Mast and Jan-Simon Schmidt). While the TXM was down, the team performed an update of the control software of the TXM and partly of the beamline. Now it runs under the latest Linux (Debian) OS, EPICS and QT versions on a new workstation. This was done at the same time as implementing a more sensitive camera for the incorporated fluorescence light microscope. Both projects were realised in the scope of Catharina Häbel's bachelor's and master's theses at Hochschule für Technik und Wirtschaft Berlin (University of Applied Sciences).

NEW FEATURES AND CAPABILITIES FOR BESSY II

With the transformation of the BESSY II light source into a **variable-pulse-length storage ring**, HZB will host the first synchrotron light source in the world to deliver brilliant X-ray pulses with user-selectable durations. This will open up new opportunities for researchers, including new studies on energy materials.

Since 1998, HZB has been operating its third-generation synchrotron light source BESSY II, which provides VUV and soft X-rays. It offers an outstanding and reliable research environment not only for researchers at HZB, who primarily use the light for research on energy materials, but also for the approximately 2000 guest researchers who travel to Berlin from all over the world each year in order to study their samples at BESSY II.

During its current regular operation, BESSY II provides brilliant X-ray pulses at a duration of 17 picoseconds (1 picosecond = 10^{-12} s). For a few days each year, it is already feasible to change the operating mode so that samples can be studied using shorter pulses of about three picoseconds. Short pulses are necessary for imaging fast atomic processes over time, for example. Up to now, though, this mode has always weakened the photon flux to only a fraction of its regular intensity.

Flagship project BESSY-VSR: With the transformation of the BESSY II light source into a variable-pulse-length storage ring, Berlin will become even more attractive as a scientific location to researchers from the world over.

BESSY-VSR will offer both short and long light pulses

The upgrade will usher in some important innovations. BESSY-VSR will offer short light pulses of two-picosecond duration as well as longer pulses of 15-picosecond duration, while maintaining the photon flux at a constant, high level – even during the shorter pulses. Users will be able to select the pulse length needed for their experiments and even combine light pulses of different durations for experiments that require it.

This will bring about advancements in energy materials research at HZB. Scientists will be able to follow, for example, how the electronic structure of reactants changes during a chemical reaction. “I am very pleased that we were able to convince the Senate of the Helmholtz Association of the project’s quality”, says Prof. Bernd Rech, acting Scientific Director of HZB. “The upgrade ensures that we will continue to operate a synchrotron light source in Berlin that meets worldwide demand.”

Superconducting high-power cavity resonators are one of the things needed to realise BESSY-VSR. The State of Berlin has made 7.4 million euros from the European Regional Development Fund (ERDF) available for setting up the SupraLab@HZB application lab, which will carry out the advanced development of these cavity resonators. Researchers will be collaborating with industrial organisations to develop the technology to the point where it is ready for incorporation into BESSY-VSR and other synchrotron light sources. A total of 29.4 million euros is being invested in the upgrading of BESSY II.

Wide approval in the expert community

The application for the project and approval from the Helmholtz Association were issued only after the topic had been discussed intensively within the expert community. HZB thus ensured the needs of users would be given central importance in the advanced development of BESSY II. The Committee Research with Synchrotron Radiation, which represents German synchrotron users, approved of the upgrade of BESSY VSR and stressed its relevance, in that BESSY VSR would add very unique capabilities to the portfolio for synchrotron users in Germany, Europe and worldwide. BESSY VSR is an essential component of the HZB Strategy 2020+, for which HZB has received the explicit agreement of the Supervisory Board and of the Helmholtz Association. *ih*

More than 2,000 guest researchers come to Helmholtz-Zentrum Berlin every year for the experimental capabilities, some of them unique in the world, of the beamlines and instruments at the light source BESSY II.

The synchrotron source BESSY II is being upgraded into a variable-pulse-length storage ring (VSR) in the scope of the HZB Strategy 2020+ project. When finished, researchers will be able to work with bright X-ray pulses of two different durations.

FACTS AND FIGURES ABOUT HZB

22

per cent of the 654 scientific employees at HZB at the end of 2017 were women. The proportion of women among all 1,155 employees was 29.3 per cent.

81

per cent of radiation time at BESSY II in 2017 was for HZB-external use.

6,584

hours (823 shifts or 274 days) were dedicated to scientific use of the storage ring facility BESSY II in 2017. This equates to 75 per cent availability. 922 hours (124 shifts or 41 days) were reserved for accelerator experiments.

252

cooperatives were maintained by HZB with other scientific establishments at the end of 2017 – a remarkable increase compared with the previous year (137).

22

young students from 15 countries worked at HZB for eight weeks during the summer of 2017 as part of the popular Summer Programme. As always, they were supervised by enthusiastic HZB researchers.

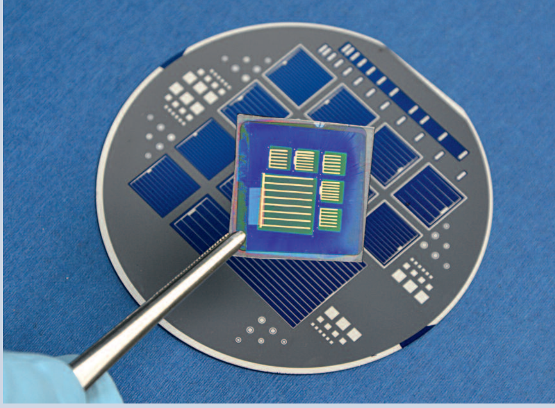
462

ISI- and SCOPUS-cited papers were published by scientists of HZB in 2017.

19.48

million euros in third-party funding went to HZB in 2017. This included around 4.96 million euros for contract research, 3.15 million euros for services for third parties, around 3.38 million euros in project funding from the Federal government, and around 3.37 million euros from the European Union.

HZB's Summer Programme is highly popular among students from all around the world. For one whole summer in 2017, 22 young people from 15 countries once again collaborated on various projects with researchers at HZB.



HZB has many research groups working on so-called energy materials. One aim is to functionalise the material class of metal–organic perovskites for solar cells.

174

PhD students were supervised at HZB in 2017. The number of theses completed in the same year was 34.

4.66

million euros were received by HZB for technology transfer in 2017. Around 1.61 million euros came from research and development partnerships and from R&D orders with domestic and international commercial enterprises, nearly one million euros from other R&D cooperatives. Another 2.09 million euros originated from infrastructure agreements.

9

young investigator groups were researching at HZB in 2017, topping the previous year's four groups. Eight of these young investigator groups are in the POF field "Renewable Energies" and the other is in the POF field "From Matter to Materials and Life".

5

patents were granted to HZB in 2017. At the end of the year, HZB's portfolio amounted to 215 patents, 26 of which are objects of ongoing licence agreements. 12 invention disclosures from 2017 were evaluated by HZB or external technology experts with regard to their patentability and/or commercial exploitability.

75

cooperative partnerships between HZB and companies were newly established in 2017 alone. Thus the total number of ongoing cooperative partnerships with industry rose considerably from 109 in the previous year to 135. Of these, nearly 30 per cent were cooperatives with companies from outside Germany and nearly 32 per cent cooperatives with small to mid-sized businesses.

149

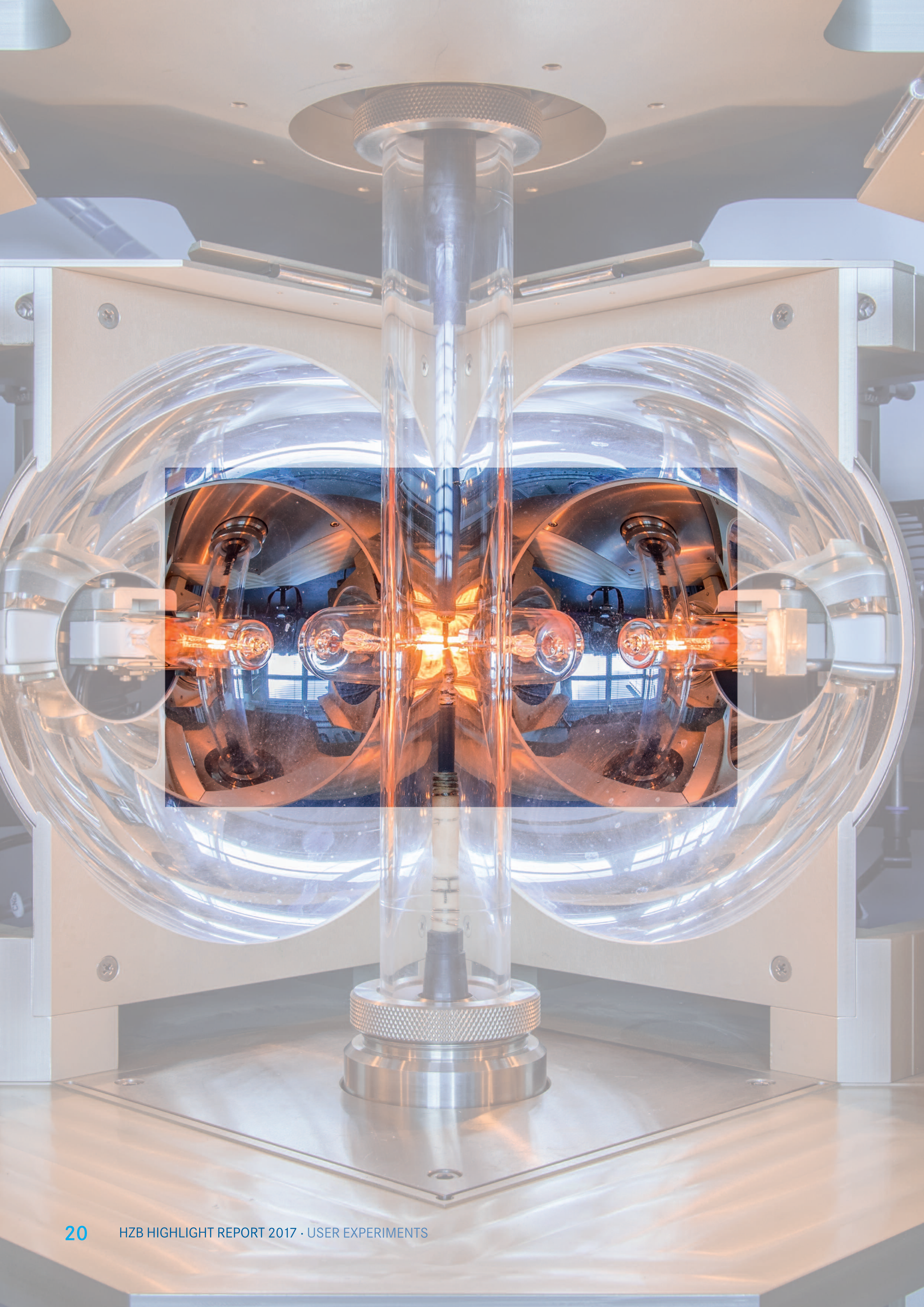
days over 13 reactor cycles were clocked for powered operation of the research reactor BER II in 2017. This equates to a total of 1,475 instrument days of regular operation on 10 instruments. 199 instrument days were needed for instrument development and maintenance. The remaining 1,276 experimental days were used for the experiments of internal and external guests.

3,000

school students experimented at the two School Labs in Wannsee and Adlershof in 2017. 60 per cent were from primary schools and the remaining students from secondary schools.

40

adolescents and young adults were receiving training at HZB at the end of 2017.



HIGHLIGHTS FROM USER EXPERIMENTS

The **Neutron time-of-flight spectrometer NEAT II** welcomed its first users in 2017. NEAT II has a long history of successful application in studying dynamics and function over very broad time and space domains, ranging from 10^{-14} to 10^{-10} seconds and from 0.05 to about 5 nanometres, respectively. Launched originally as NEAT I, the upgrade started in 2010 after a rigorous internal and external selection process, and resulted in 70-fold higher flux and a number of new instrumental capabilities including greater angular resolution, a larger accessible wavelength range and a design suitable for high magnetic field experiments of up to 15 teslas.

The **CoreLab Quantum Materials**, established in 2017, is already HZB's sixth CoreLab for researching energy materials. A research team from the HZB Institute for Quantum Phenomena in New Materials, led by Prof. Dr. Bella Lake and Dr. Konrad Siemensmeyer, has set up the CoreLab and its modern equipment and is also responsible for it. External researchers are also welcome to use this CoreLab and to benefit from the expertise of the HZB team.

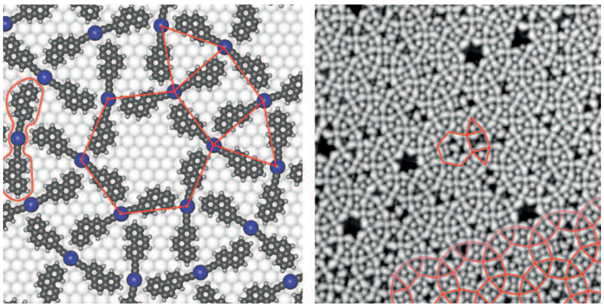
The **research project CALIPSOplus**, being funded with 10 million euros from the EU and in which HZB is also involved, officially started in 2017. The project has a runtime of four years and is aimed at promoting the international exchange of scientists and transnational access to the 19 participating light sources in Europe. In the scope of CALIPSOplus, HZB manages the work package "Dissemination and Training" and is involved in the research project MOONPICS on the metrology of nanometre lenses.

In 2017, the **Energy-Materials In-Situ Laboratory Berlin (EMIL)** successfully guided X-rays all the way from Undulator UE48 in the BESSY II experimental hall to the EMIL laboratory and its CAT experiment. There, it was quantitatively measured using a focus measuring chamber. All parameters important for later experimental operation such as beam diameter (108 x 56 μm^2), photon flux (approx. $10^{12\ s^{-1}}$) and resolution (50 meV at 400 eV) satisfied and met the expectations and calculated values. The beamline thus promises to be one of the most powerful of its kind in this energy range.

SIMPLE ORGANIC MOLECULES FORM COMPLEX MATERIALS

An international team of researchers lead by the Technical University of Munich (TUM) has discovered a chemical reaction pathway that produces **exotic layers with semiregular structures from simple two-dimensional networks**. Materials researchers can use this to develop new materials with extraordinary properties.

Only a few basic geometric shapes lend themselves to covering a surface as uniformly shaped tiles without overlaps or gaps: triangles, rectangles and hexagons. Considerably more and significantly more complex regular patterns are possible by combining two or more tile shapes. These are so-called Archimedean tessellations or tilings. Materials can also exhibit tiling characteristics. These structures are often associated with very special properties, for example unusual electrical conductivity, special light reflectivity or extreme mechanical strength. However, producing such materials is difficult. It requires large molecular building blocks which are not compatible with traditional manufacturing processes.



The new building block (left, red outline) comprises two modified starting molecules connected to each other by a silver atom (blue). This leads to complex, semiregular tessellations (right, microscope image).

Complex tessellations through self-organisation

An international team led by Prof. Florian Klappenberger and Prof. Johannes Barth at the Chair of Experimental Physics of TUM, as well as Prof. Mario Ruben at the Karlsruhe Institute of Technology, have now made a breakthrough in a class of supramolecular networks: they got organic molecules to combine into larger building blocks with a complex tiling formed in a self-organised manner. As a starting compound, they used ethynyl iodophenanthrene, an easy-to-handle organic molecule comprising three coupled carbon rings with an iodine and an alkyne end. On a silver substrate, this molecule forms a regular network of large hexagonal meshes. Heat treatment sets a series of chemical processes in motion, producing a novel, significantly larger building block which then forms a complex layer with small hexagonal, rectangular and triangular pores virtually automatically and self-organised. In the language of geometry, this pattern is referred to as a semiregular 3.4.6.4 tessellation.

Molecular reorganisation observed at BESSY II

"The scanning tunnel microscopy measurements we conducted at TUM show clearly that the molecular reorganisation involves many reactions that would normally result in numerous by-products. In this case, however, the by-products are recycled, meaning that the overall process runs with great economy of atoms – nearly one hundred per cent recovery – to arrive at the desired end-product", explains Klappenberger. The researchers revealed precisely how this happens in further experiments. "Using X-ray spectroscopy measurements at the electron storage ring BESSY II of the Helmholtz-Zentrum Berlin, we were able to decipher how iodine splits from the starting product, hydrogen atoms move to new positions and the alkyne groups capture the silver atom", explains lead author Yi-Qi Zhang.

By way of the silver atom, two starting building blocks bind together to create a new, larger building block. These new building blocks then form the observed complex pore structure. "We have discovered a completely new approach to producing complex materials from simple organic building blocks", summarises Klappenberger. "This is important for the ability to synthesise materials with specific novel and extreme characteristics. These results also contribute to better understanding the emergence or spontaneous appearance of complexity in chemical and biological systems."

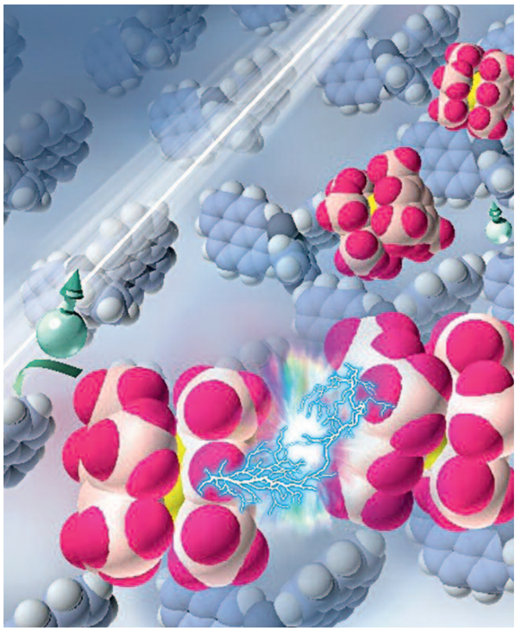
arö/TUM

Nature Chemistry, 10, 296–304, 2018 (DOI:10.1038/nchem.2924): Complex supramolecular interfacial tessellation through convergent multistep reaction of a dissymmetric simple organic precursor, Yi-Qi Zhang, M. Paszkiewicz, P. Du, L. Zhang, T. Lin, Z. Chen, S. Klyatskaya, M. Ruben, A. P. Seitsonen, J. V. Barth, and F. Klappenberger

LIGHT FACILITATES NEGATIVE DOPING OF ORGANIC SEMICONDUCTORS

Using a two-step process, a German-American research team has managed to increase the **conductivity of an organic semiconductor** considerably. Possible applications include light-emitting diodes and solar cells

Semiconductor devices are omnipresent – not just in microchips, but also in solar cells that convert light into electrical energy, and in many other applications that are part of daily life. Organic semiconductor materials have also been the subject of increasing research and development over the past few years. Their electrical properties can also be changed by the intentional incorporation of a tiny number of foreign atoms or molecules that enable their conductivity to be precisely set. This is done in a process known as "doping", where positive (p) or negative (n) molecules are introduced into the material.
However, for modern applications, one needs both p-doped and n-doped semiconductor layers, as they are called, combined in the one device. N-doping of organic semiconductors is extremely difficult, though. The class of organic molecules employed for n-doping reacts readily with oxygen and water, which are present in normal environmental conditions.



The illustration shows how photons break the dimers into the individual organometallic molecules again, which then effectively n-dope the organic semiconductor.

Two steps for n-doping

A German-American team has demonstrated a new approach for doping organic semiconductors with n-type donor molecules. Groups from the Georgia Institute of Technology, Princeton University, Humboldt-Universität zu Berlin, and HZB joined forces for this work.
The new approach consists of two primary steps. In the first step, organometallic molecules, the n-dopants, are connected into what is referred to as a dimer. This molecular couple is far more stable compared to the individual dopant molecules, and can be easily incorporated into the organic semiconductor; however, the dimer itself is not suitable as an n-dopant and does not release any negative charges. The revolutionary second step involves shining light on the mixture. In a multi-stage chemical process, the incident photons break the dimers apart again into their individual organometallic molecules, which then effectively n-dope the organic semiconductor.

Increased conductivity and lifetime

"By activating the dopants with light, we were able to increase the conductivity of organic semiconductors by five orders of magnitude. This could considerably increase the efficiency of organic light-emitting diodes and solar cells", says Prof. Antoine Kahn from Princeton University, who coordinated the project. "Our approach enables far simpler manufacturing of n-doped organic semiconductor materials used in diverse applications. The critical step in the process – that of breaking the dimers with light to activate doping – can be done after encapsulation so that the active dopant molecules are never exposed to air. This will also increase the operating lifetime of devices that rely on n-doped layers", explains Prof. Norbert Koch, who heads the joint Molecular Systems research group of HU Berlin and HZB.

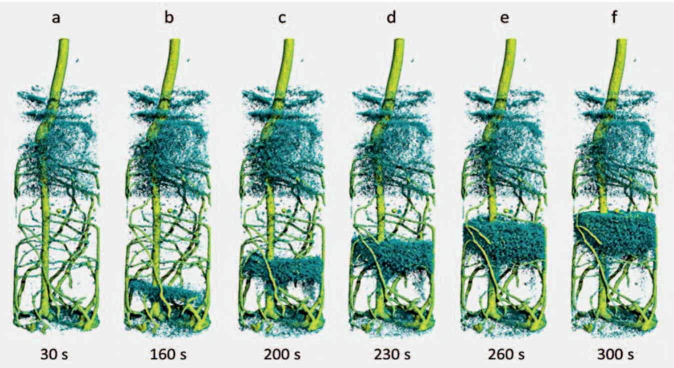
red/arö

Nature Materials, 16, 1209–1215, 2017 (DOI: 10.1038/nmat5027): Beating the thermodynamic limit with photo-activation of n-doping in organic semiconductors; X. Lin, B. Wegner, K. Min Lee, M. A. Fusella, F. Zhang, K. Moudgil, B. P. Rand, S. Barlow, S. R. Marder, N. Koch, and A. Kahn

LUPIN ROOTS OBSERVED IN THE ACT OF CATCHING WATER FROM SOIL

A team of the University of Potsdam, working with the HZB imaging group at BER II, has improved the **temporal resolution of neutron tomography** more than a hundred-fold.

Soil scientists led by Prof. Sascha Oswald from the University of Potsdam regularly conduct experiments at the BER II neutron source. This is because neutrons are superbly suited to observing the transport of water in soil and plant roots. To study a lupin plant, they place the root in a column of soil and rotate it slowly but continuously as they take very fast snapshots of it. The team is now able to conduct a full 3D mapping in only ten seconds, instead of one hour, thanks to specific technical modifications at the CONRAD-2 imaging facility made by HZB experts Dr. Nikolay Kardjilov and Dr. Ingo Manke. These modifications enabled the researchers from the University of Potsdam to observe for the first time in 3D how water rises upwards in the soil and thus how the roots absorb it. “At this temporal resolution it had only been possible thus far to look at the sample cross-section radiographically, i.e. in 2D”, explains Dr. Christian Tötzke, first author of the study. The findings extend our understanding of the interactions between roots and soil, which is also relevant for the breeding and cultivation of these kinds of agricultural crops. And the new recording technology, which is a good one hundred times faster than before, could also enable rapid processes in fuel cells, batteries, and construction materials to be observed in real time. *arö*



Sequential tomography of a lupin root (yellowish green) after deuterated water (D2O) was introduced from below. The rising water front (H2O, dark blue) is displaced by the D2O from below over the course of time. The complete sequence can be viewed as a video.

Scientific Reports, 7, 6192, 2017 (DOI: 10.1038/s41598-017-06046-w): Capturing 3D Water Flow in Rooted Soil by Ultra-fast Neutron Tomography; C. Tötzke, N. Kardjilov, I. Manke, S. E. Oswald.

TUNEABLE OPTICAL PROPERTIES OF GRAPHENE

A research team has for the first time investigated the optical properties of three-dimensional nanoporous graphene, which could be used for highly sensitive chemical sensors, at the IRIS infrared beamline of BESSY II.

A team led by a group at Sapienza University in Rome was able to ascertain how charge density oscillations, known as plasmons, propagate through three-dimensional graphene. In doing so, they determined that these plasmons follow the same physical laws as in 2D graphene. However, the frequency of the plasmons in 3D graphene can be very precisely controlled, either by introducing atomic impurities (doping), by changing the size of the nanopores, or by attaching specific molecules in certain ways to the graphene. Furthermore, the new material is promising as an electrode material for use in solar cells. “A special operating mode of the BESSY II storage ring, called low-alpha, allowed us to measure the optical conductivity of three-dimensional graphene with a particularly high signal-to-noise ratio. This is hardly possible with standard methods, especially in the terahertz region. However, it is exactly this region that is important for observing critical physical properties”, says Dr. Ulrich Schade, head of the group at the infrared beamline. *arö*

Nature Comms., 8, 14885 (DOI: 10.1038/ncomms14885): Terahertz and mid-infrared plasmons in 3D nanoporous graphene; F. D’Apuzzo et. al.

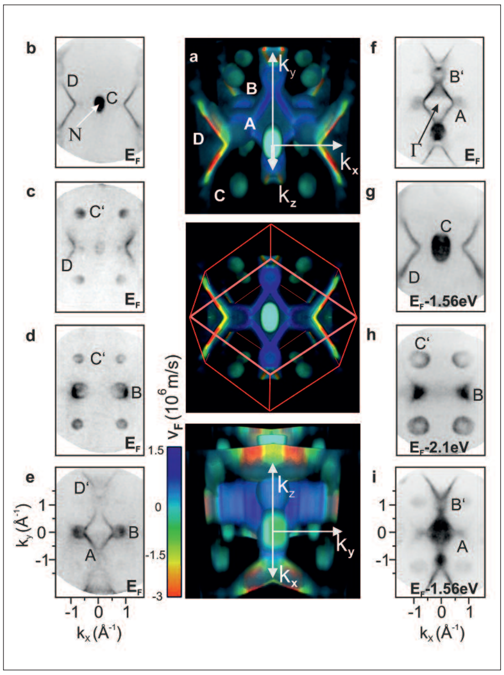
A MAP OF THE FERMI SURFACE

By combining experiments in different spectral ranges, scientists at HZB succeeded in precisely mapping the **electronic structure of tungsten**. This opens up new perspectives for innovative tailored materials.

Researchers around the world are always looking for new kinds of materials. A common aim is to create materials with extraordinary electronic properties. These would be used to create highly sensitive magnetic field sensors or components for future spintronics, for example – a new form of data processing based on the spin of electrons. One very promising class of materials is the so-called topological insulators. These are solids whose surface allows current to flow but whose internal bulk completely insulates electric currents and fields.

If we are to develop materials like these with tailored characteristics for specific applications, we need a precise understanding of the electronic and thermal properties of their constituents. These properties, in turn, depend on two distinguishing physical parameters above all others: the Fermi surface and the Fermi velocity – mathematical constructs physicists use to describe the energy states of the electrons in a metal. "In a topological insulator, the number of times an energy band crosses the Fermi surface tells us what kind of insulating properties it can have," says Dr. Katarina Medjanik, who researches such materials at the Institute of Physics at Mainz University.

Together with a team from seven research institutions in Germany, Great Britain and Switzerland, the physicist succeeded for the first time in directly mapping the electronic structure on the Fermi surface in tungsten. To achieve this, the team used instruments at the accelerator facility PETRA III of DESY in Hamburg and at BESSY II.



Images that tell physicists a great deal: the experimentally elucidated structure of the Fermi surface and distribution of Fermi velocities in tungsten. Knowledge of these structures helps researchers in developing new, tailored materials.

Detailed insights thanks to BESSY II

"We began our experiments in 2015 at BESSY II, using low-energy ultraviolet radiation," the researcher from Mainz recounts. The researchers also employed a method called time-of-flight momentum microscopy, which had been newly developed at Mainz University and at the Max Planck Institute for Microstructure Physics in Halle. The team combined the insights they gained through this with measurements in soft X-ray light at the accelerator in Hamburg. "This combined method, used for the first time worldwide, ultimately led to success," says Medjanik. The capabilities offered at HZB helped especially. "The experiments there delivered highly detailed and comprehensive information about the electronic system we were studying – and at the same time caused hardly any radiation damage to the material," the physicist explains. Expert colleagues who reviewed the paper before it was published in Nature Materials described the result as a "breakthrough", she proudly reports.

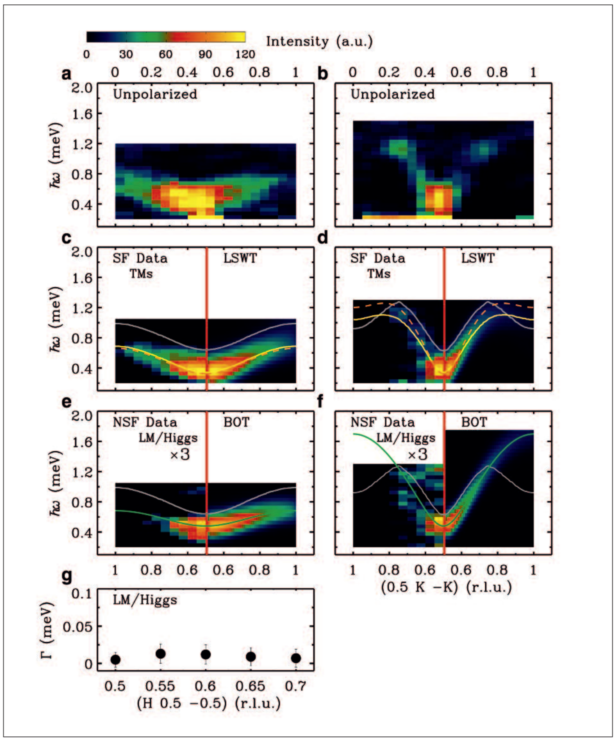
"We showed for the first time that all essential parameters such as the Fermi surface and the distribution of Fermi velocity can be derived from the measurements," Medjanik explains. The experiments in Hamburg and Berlin also revealed, to the researchers' surprise, that "topological states" exist on normal metallic surfaces. A rather obscure-sounding discovery, perhaps, but this opens up new possibilities for materials scientists to design exotic materials with potential for exciting applications. *rb*

Nature Materials, Vol 16, 2017 (DOI: 10.1038/nmat4875): Direct 3D mapping of the Fermi surface and Fermi velocity; K. Medjanik et. al.

HIGGS-LIKE QUASIPARTICLE IN A SPIN SYSTEM

Some of the **bizarre effects known from elementary particle physics** can also be found in solid bodies. An international research team has now directly observed one of these experimentally elusive phenomena.

The name Higgs boson carries an air of weighty importance in physics. Scientists spent decades hunting for the Higgs boson – an originally hypothetical elementary particle of momentous importance in the standard model of particle physics. The particle, named after British physicist Peter Higgs, embodies a mysterious field that lends other particles their mass. The theory was developed in the 1960s, but it took until 2012 before researchers at CERN, the European Organization for Nuclear Research in Geneva, finally found the particle.



Scoping out spin dynamics with polarised neutrons: these false-colour pictures show the spectra of magnetic excitations as a function of energy and momentum exchange – as well as various analyses of the experimental data. This gives researchers an insight into quantum phenomena occurring in the studied sample.

Shy particles in a quantum material

Physicists have recognised that the Higgs boson's properties are not entirely unique. Effects have also been observed in solid-state physics that bear a resemblance to the mechanism of how particles acquire their mass. In superconducting materials, particles can appear that behave similarly to the Higgs boson. The theory predicts the existence of similar entities in other quantum systems, too – for example in so-called quantum antiferromagnets. A quantum phase transition in these special magnets can create the best condition to observe "Higgs amplitude modes". These are shy quasiparticles which normally decay very rapidly into other particles.

A team of scientists led by US physicist Dr. Tao Hong of Oak Ridge National Laboratory in Tennessee has succeeded in truly observing this exotic quantum material state. The researchers worked with a metal-organic compound abbreviated as DLCB, composed of copper ions and ideal for studying exotic quantum effects. Under specific conditions, the spins in this material arrange themselves into a flat, regular lattice resembling two-dimensional coupled ladders.

Excitation with cold neutrons

Hong and colleagues studied exotic quantum effects and analysed low-energy excitations in DLCB using inelastic scattering of "cold" neutrons – a method in which low-energy neutrons invoke crystalline states in the studied material. The researchers performed one part of the experiment on the three-axis neutron spectrometer FLEXX at BER II.

As a stroke of luck for the researchers, the quantum mechanical energy gap in DLCB proved to be of a special kind. It namely prevented the Higgs quasiparticle from rapidly decaying as it normally would in most other materials. This gave them enough time to prove the existence of the curious entity beyond a doubt, and even measure its characteristics. The results are especially exciting for basic research because they allow a hitherto impossible look at the properties of exotic quantum materials. *rb*

Nature Physics, Vol 13, 2017 (DOI: 10.1038/nphys4182): Higgs amplitude mode in a two-dimensional quantum antiferromagnet near the quantum critical point; T. Hong et. al.

PENETRATING INSIGHT INTO A BEETLE FOSSIL

In the **high-resolution light of the Berlin synchrotron source BESSY II**, researchers have identified an insect trapped in amber. Its lineage is betrayed by the features of the genitalia.

Minute scavenger beetles exist in many forms all over the world. Around 800 species of some 30 genera are currently known. But even more species once used to exist in this beetle family, known to experts under the scientific name of *Latridiidae*. Researchers have so far discovered nearly two dozen extinct species. Many of these fossils have been found encapsulated in airtight amber from the Baltic Sea region. A team of scientists has successfully identified a new species using modern X-ray spectroscopy at BESSY II.

"Some species of *Latridiidae* are only distinguishable after detailed examination of the male genitalia," says entomologist Dr. Hans-Peter Reike from Chemnitz, who has been researching beetles for many years. "Minute scavenger beetles belong to the genus of *Corticaria*." The first amber-fossilised remains of a minute scavenger beetle in this genus were discovered in 1845. The beetle specimen Reike and the team of researchers from HZB examined, using an analytical method that is so far unique, is trapped in a two-millimetre-thick piece of amber about the size of a fingernail. It is fully intact and only has two fine cracks in the encapsulating material running through it. "The insect clearly belongs to the subfamily *Corticariinae*, which is distinguishable by certain physical features," the researcher from Chemnitz explains. Specifically, it possesses a smooth head without furrows or ridges, the front coxae are not widely separated and the sides of the pronotum have a finely toothed edge.

Teensy structures in 3D

In order to find out which species of minute scavenger beetle the fossil belongs to, the scientists scanned the insect and its surrounding amber with X-ray light from the synchrotron radiation source BESSY II. What is special about this is that "unlike the radiation from conventional X-ray sources, the X-ray light from the synchrotron lets you produce high-resolution and, even more importantly, high-contrast pictures in so-called phase-contrast mode," explains Dr. Ingo Manke, a researcher at the HZB Institute of Applied Materials. In addition to measuring the amplitude of the light waves, it also measures their phase, or in other words the temporal shift in the periodic sequence of wave peaks and troughs. "The phase-contrast method is helpful above all in studying samples that contain light chemical elements," Manke says – such as carbon, which makes up most of the insect's exoskeleton.

By X-raying the beetle on HZB's tomography instruments, the researchers were able to resolve even the teensiest of structures at around one micron in size. They took many separate shots and then used a special software program to stitch them into an extremely sharp, three-dimensional picture of the fossil. "The morphology of the male genitalia was then clearly discernible," Reike says. A stroke of luck for the researchers, it turns out: it allowed them to classify the beetle easily into a new, hitherto unknown species.

rb

Ventral view of the minute scavenger beetle of the subfamily *Corticariinae*, which was able to be identified with the help of high-resolution light from the synchrotron source BESSY II.

Zootaxa, 4242 (3), 578-590 (DOI: 10.11646/zootaxa.4242.3.9): Phase-contrast synchrotron microtomography reveals the internal morphology of a new fossil species of the *Corticaria-sylvicola*-group (Coleoptera: Latridiidae); H.-P. Reike, A. Bukejs, T. Arlt, N. Kardjilov, and I. Manke

JOINT RESEARCH GROUPS

HZB AND **FREIE UNIVERSITÄT BERLIN** ARE ESTABLISHING GROUPS FOR “MACROMOLECULAR CRYSTALLOGRAPHY” AND “X-RAY MICROSCOPY”.

For many years, HZB’s “Macromolecular Crystallography” work group has been successfully cooperating with the “Structural Biochemistry” research group headed by Prof. Markus Wahl at Freie Universität Berlin. Since 2017, they have intensified this cooperation within the framework of a joint research group dedicated to studying the biochemistry of genetic information processing. This research group benefits in particular from access to the three MX beamlines where it can study protein crystals using the synchrotron light from BESSY II. HZB is primarily working on enhancing the instrumentation and methodological aspects of macromolecular crystallography, while the group of Freie Universität Berlin is introducing its expertise in the field of structure–function relationships in gene regulation.

Also in 2017, the joint research group “X-Ray Microscopy” was launched, combining the expertise of teams led by Prof. Gerd Schneider at HZB and Prof. Helge Ewers at Freie Universität Berlin. While Ewers’ group contributes its experience in the field of optical microscopy and biological research, the HZB work group is responsible for X-ray microscopy at the synchrotron source BESSY II. Optical microscopy and super-resolution methods are excellent for locating proteins marked with dye molecules in tissue samples. X-ray microscopy, in turn, allows correlative imaging of the distribution of proteins, viruses or nanoparticles over a relatively large section in high-resolution and three dimensions. The two microscopy methods thus deliver a comprehensive picture of the intracellular structures and processes.

KICK-OFF FOR JOINT LAB WITH IFW DRESDEN

The Leibniz Institute for Solid State and Materials Research Dresden (IFW) and HZB have created the Joint Lab “Functional Quantum Materials”. This joint lab will take advantage of both institutes’ long-standing expertise in energy and materials research, and in the growth of epitaxial films. The new lab is dedicated to exploring new materials with promising quantum properties for future applications, for example in information technologies.

With the joint lab, IFW Dresden and HZB are intensifying their collaboration in research and the promotion of young scientists. The scientists will be upgrading the common instrumentation at BESSY II with unique properties – some without rival in the world. A Young Investigator Group, headed by Dr. Alexander Fedorov, has also been established under the umbrella of the joint lab.

HZB AND THE MAX PLANCK SOCIETY ARE BUILDING THE BELCHEM LAB

Helmholtz-Zentrum Berlin is establishing a joint lab together with the Max Planck Society (MPG) for studying electrochemical phenomena at solid/liquid interfaces. The Berlin Joint Lab for Electrochemical Interfaces, BElChem, will employ X-rays from BESSY II to analyse materials for renewable energy production. The partners will operate three dedicated beamlines at the BElChem Joint Lab, two of which will generate soft X-rays and one that will provide hard X-rays. “We are creating an ideal environment at BElChem for detailed investigations of electrochemical processes in complex systems of materials under realistic conditions. For example, we want to analyse how artificial leaf systems work in splitting water molecules with sunlight and generating hydrogen”, says Prof. Roel van de Krol, who heads the HZB Institute for Solar Fuels.

NEW RESEARCH PROJECT WITH AVANCIS

THE GOAL IS TO IMPROVE THE OUTDOOR PERFORMANCE OF **THIN-FILM CIGS SOLAR MODULES.**

The Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin (PVcomB) at HZB is contributing its expertise to improving copper-indium-gallium-sulphide (CIGS) thin-film production in the MyCIGS collaborative research project. CIGS-module manufacturer AVANCIS in Munich is coordinating this project funded by the German Federal Ministry for Economic Affairs and Energy (BMWi). The Carl von Ossietzky University of Oldenburg (Oldenburg University) and Friedrich-Alexander-Universität Erlangen-Nuremberg (FAU) are also partners in the project.

The energy yields of CIGS modules under real-world conditions can be measured on an outdoor testing platform at PVcomB.

Thin-film solar modules based on CIGS are highly efficient, economical and versatile. Thanks to their special properties, they can be employed not only on rooftops, but in building cladding as well. Building-integrated photovoltaics (BIPV) offers diverse new aesthetic configurations for architecture and will find a place on many more surfaces to come in urban environments.
Whereas module efficiency has been the focus of previous projects, the MyCIGS project will address how to optimise the energy yield in real-world applications, i.e. under realistic conditions of outdoor use. In addition to efficiency, properties such as temperature coefficients and power output under conditions of low or diffuse illumination are critical factors. These also play an important role when employing CIGS modules in cladding and building structures. “We have a lot of experience at PVcomB with characterising and tuning the performance of CIGS thin-films”, explains Dr. Reiner Klenk, in charge of the MyCIGS Project at PVcomB. Using the numerous measurement techniques that have been established at PVcomB, major parameters such as temperature coefficients and behaviour under low-light conditions can be traced back to physical processes in the solar module. The research project fits in with PVcomB’s strategy of going beyond manufacturing technologies to address other topics such as encapsulation, reliability, outdoor measurements and building integration.
As part of the Helmholtz Energy Systems Integration Project for the Future, a new research group headed by Dr. Carolin Ulbrich has just been established. This research group will now be able to measure the energy yields of CIGS modules and to acquire data sets on local incident radiation and temperature by means of an outdoor testing platform at PVcomB.

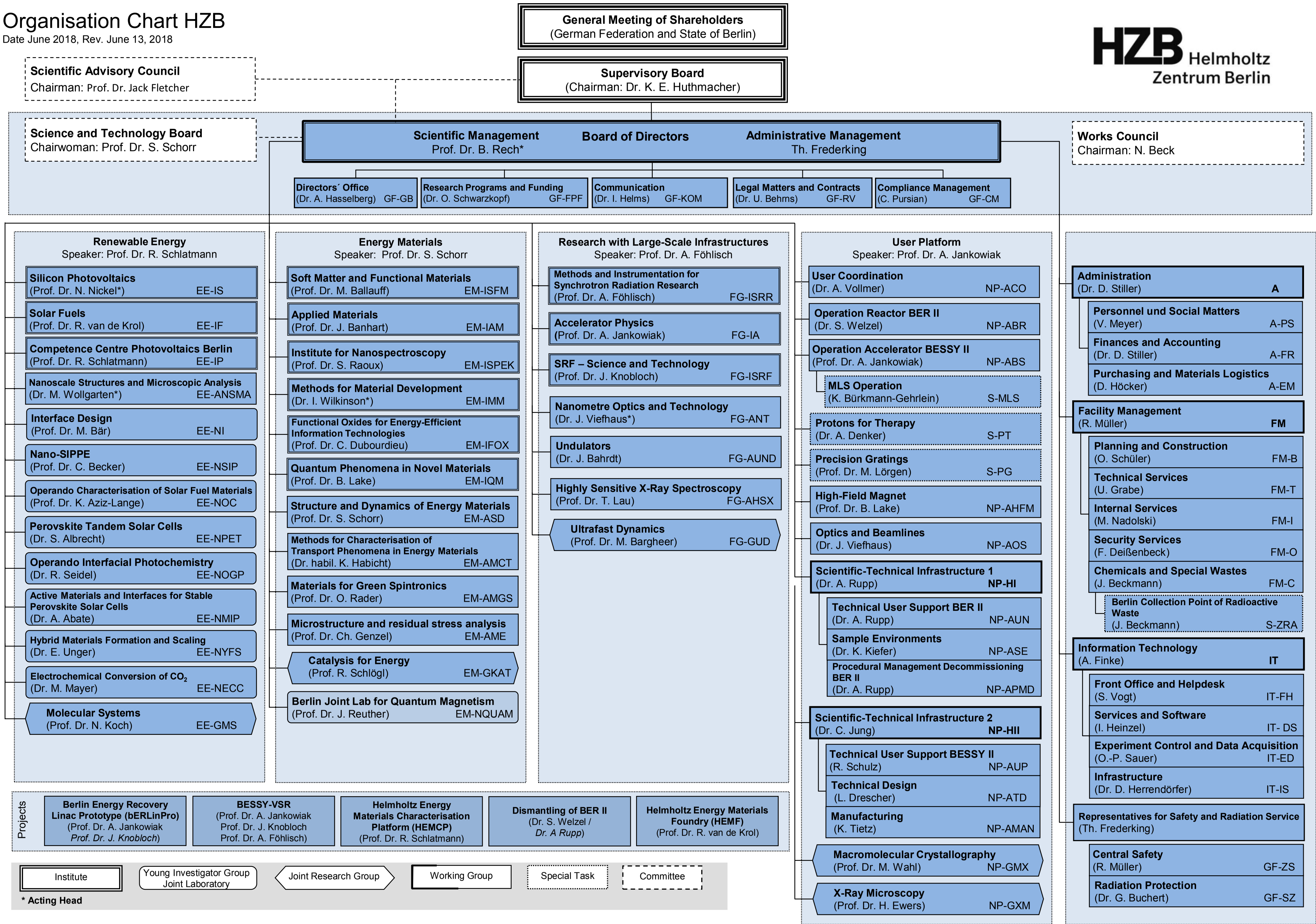
IMPORTANT APPOINTMENTS

Prof. Dr. Christiane Becker, head of the Young Investigator Group “Nanostructured Silicon for Photonic and Photovoltaic Implementations”, has accepted the call to a permanent W2 professorship for the field of “Experimental physics focusing on material sciences and photonics” at HTW Berlin University of Applied Sciences. She had already been called to a temporary W2 professorship at HTW Berlin in 2014.

Prof. Dr. Catherine Dubourdieu, head of the HZB Institute “Functional thin film oxides for energy efficient future information technology”, received a W3 professorship at Freie Universität Berlin from a joint appointment procedure in December 2017. The physicist is an expert in the field of functional metal oxides that are promising candidates for future information technologies.

Organisation Chart HZB

Date June 2018, Rev. June 13, 2018



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.

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