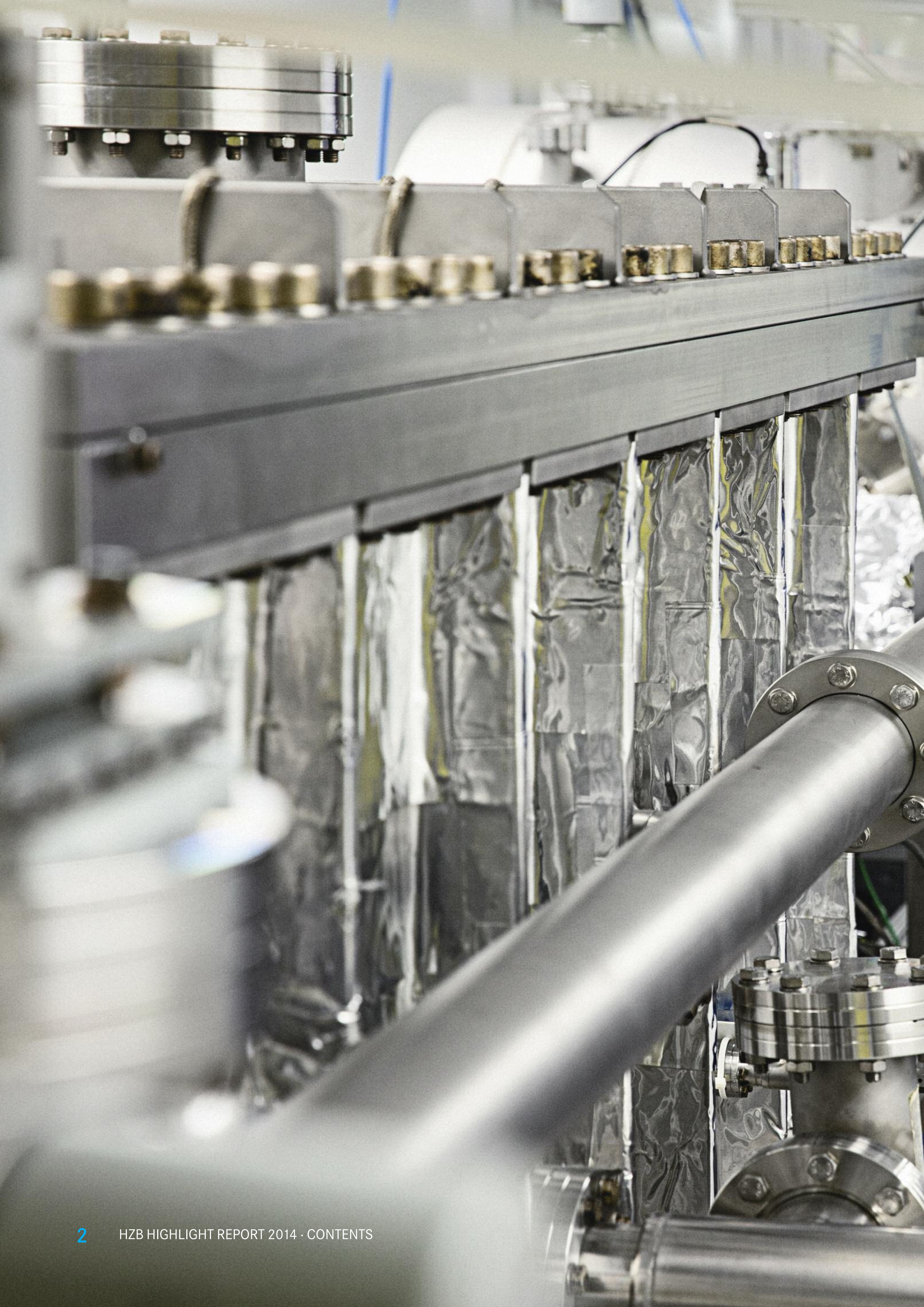
HZB Helmholtz Zentrum Berlin

FOCUSSING ENERGY REALISING VISIONS

HIGHLIGHTS 2014

Annual report with research highlights at the

Helmholtz-Zentrum Berlin für Materialien und Energie



CONTENTS

INTO THE FUTURE WITH A TAILWIND

In the spring of 2014, the reviews conducted for the programme-oriented funding (POF) were barely finished before folks at the HZB had to prepare for the next evaluation. This time, the review looked beyond the POF and at the strategy for the years beyond 2020. Once again, as from the POF review, the HZB received an extremely positive appraisal – and affirmation that we are on the right track!

This positive appraisal coming immediately from the Future Review Panel means a great deal. The Panel was contractually formed in 2009 when the former Hahn-Meitner-Institut (HMI) fused with BESSY GmbH to the new HZB. Two years ago, once the date for powering down the neutron source BER II had been announced, the shareholders agreed the Future Review Panel would be set into action in 2015. Its task, upon expiry of the HZB's first POF period and the start of the next five-year period, was to review the HZB's future plans for the years beyond 2020.

Prof. Dr. Anke Kaysser-Pyzalla and Thomas Frederking.

So it was crucial that the HZB present a strategy beyond the five-year plan of the Helmholtz Association's programme-oriented funding. This we achieved splendidly. It means we have a strong tailwind as we embark on our path to the future. This path will surely bring many new things. And we have a strong foundation on which to build. The Future Review Panel, for example, has backed our decision to continue focusing our in-house research on energy materials. The path we took in preparation for the previous POF review turned out to be the right one. Be it topological insulators, graphene, silicon or metal oxides, there are many thin-film systems that play a role in energy conversion and storage, or fulfil certain functions with high energy efficiency. Researching into the physical phenomena behind these functions is profoundly important to our scientists. We will accordingly continue to expand our portfolio of energy-related thin-film systems in the future.

> "The Future Review Panel has backed our decision to continue focusing our in-house research on energy materials. The path we took in preparation for the previous POF review turned out to be the right one."

The HZB – following the recommendations of the Future Review Panel – will be merging photovoltaic research activities increasingly with solar fuel research. Most notably, the Panel has encouraged us to combine our energy research with the capabilities of BESSY-VSR. This is no trivial forward-looking statement, for we also have the Panel's mandate to "realise the ambitious BESSY-VSR concept".

This is exactly what we are doing now. At the end of June 2015, we submitted the implementation application for BESSY-VSR to the Initiative and Networking Fund of the Helmholtz Association as a strategic expansion investment. In this Highlight Report, you can read an interview with Andreas Jankowiak, in which he explains what is special about BESSY-VSR and what challenges we face with this project (page 6/7).

This issue of our Highlight Report portrays many facets of the HZB that are already important cornerstones of our identity, for example our junior groups and joint labs, which we operate together with other university partners. Networking the HZB within the national and international research landscape is important and is one of the reasons why the HZB already enjoys an excellent reputation in the scientific community – a mere six years after its foundation. This networking is an essential part of our future strategy. Other achievements during the period covered in this report include gaining new joint labs, expanding our young scientists training programme, and successfully attracting visiting researchers to the HZB (pages 36, 50, 53).

> “Networking the HZB within the national and international research landscape is important and is one of the reasons why the HZB already enjoys an excellent reputation in the scientific community – a mere six years after its foundation.”

Stories from the “In-House Research” chapter on pages 22 to 35 bear testimony to the incredibly exciting topics in materials research that our HZB researchers are working on. Many of the results presented here have been published in prestigious scientific journals. They define the profile of the HZB. Alongside these, you will find other exciting stories in the “User Experiments” chapter (pages 8 to 21). In 2014, we were able to chalk up more than 3,400 user visits to BESSY II. After its long service interruption, the neutron source BER II resumed operation in the spring of 2015, meaning we will have figures for you by the next Highlight Report. We are especially excited that the world’s strongest magnet for neutron scattering experiments is now also operational. With a magnetic field of 26 teslas, as measured during trial operation, it exceeds our expectations. We can hardly wait for the first neutron experiments to be performed with it. Perhaps we will already have reports on these to include in our next Highlight Report.

In the “User Experiments” chapter, you will also find topics that go beyond the HZB’s in-house research profile. We will continue to see many external topics studied at our facilities in future. The examples on protein structure analysis or art history research attest to our excellent experimental environment for such topics as well, including an extensive laboratory infrastructure. The supervising scientists for the HZB beamlines do everything they can to ensure visiting users receive optimal service at both BESSY II and BER II, and return home with meaningful results from successful experiments. The high demands we personally place on our user service will continue to be an integral part of the HZB’s philosophy in the years to come.

We hope you enjoy reading through our Highlight Report 2014 and, at the same time, we recommend you take a look at the HZB Future Logbook *www.hzbzlog.com*. If you would like to share our enthusiasm for user service with a twist and a dash of self-irony, then take a few minutes to watch our “Happy Undulator” short at *www.youtube.com/watch?v=cvp0HrHZUDY*.

Prof. Dr. A. Kaysser-Pyzalla
Scientific Director

Thomas Frederking
Administrative Director

A UNIQUE CONCEPT WORLDWIDE

With the BESSY-VSR project, the HZB synchrotron radiation source will be upgraded into a variable-pulse-length storage ring. Once complete, scientists will be able to choose freely whether to study their samples with relatively long or with very short light pulses of high-intensity light. **Prof. Andreas Jankowiak**, head of the Institute for Accelerator Physics at the HZB, describes in an interview the technical challenges along the path towards BESSY-VSR.

Professor Jankowiak, what does VSR stand for and what is the principle behind your project?
VSR stands for Variable-pulse-length Storage Ring. At the moment, the BESSY II storage ring has 400 electron packets, all of the same length, circulating in it. The light pulses these packets give off have a high photon density and a duration of about 20 picoseconds. Only during two weeks a year do we switch to low-alpha mode, where we have shorter electron packets in the ring. This operating mode is only of interest to users who need very short light pulses of 3 picoseconds for measuring at high temporal resolution or for producing terahertz radiation. The light intensity, however, is much lower than in normal mode. VSR signifies a revolution: It will allow us to maintain both long and short electron packets in the ring when in normal mode. That means long and short light pulses will be permanently available at each measuring station – all at the same light intensity. Users can then pick whichever they need. In particular, researchers who need short pulses are excited by our concept, since it is unique in the world.

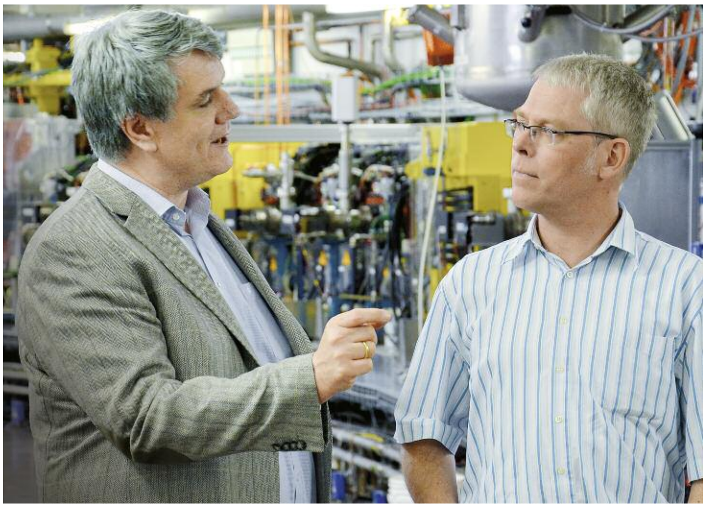
Prof. Dr. Andreas Jankowiak heads the Institute for Accelerator Physics at the HZB and is responsible for the BESSY-VSR project.

What are the next steps on the path towards BESSY-VSR?
We finished the technical design study (TDS) in March 2015. That is the concept in which we describe the challenges of the accelerator physics. And we show what needs to be done technically to realise VSR. Our Machine Advice Committee reviewed the TDS and confirmed that the assumptions are realistic. In principle, there are no reasons why anything should stand in our way – on the contrary, the mood was almost euphoric. The HZB will now apply for funding of the VSR in the scope of the strategic investments within the Helmholtz Association. Then comes another review – and if all goes well, we will have the financial commitment in 2016.

So far so good for the financing. But I suppose the components for VSR aren't exactly lying around in stock.
No, first we have to develop and test the technical solutions we have sketched out in the TDS and bring them to application maturity. We have a lot of irons in the fire. Most important will be the superconducting high-frequency cavities that shorten the electron packets. We need two pairs of these, each working at different frequencies, for producing the long and short electron packets. First, we want to develop the cavity pair for 1.5 gigahertz. This will take a lot of research work, and we need to learn a lot about technology and accelerator physics. Once the first prototype is underway, we will begin developing the 1.75-gigahertz cavities. But the 1.5-gigahertz cavities will be the first to be installed into the ring. We have to test out their effect on the electron beam. Some additional offers for user operation are conceivable. Otherwise, these two cavities will be muted – until the second, 1.75-gigahertz pair is ready for operation.

And once the cavities are in place, it's done?

There is a lot more to it than that. We need more components for the beam generation and guidance. Novel high-frequency transmitters, for example. These are necessary for creating the electromagnetic fields for accelerating the electrons. But we also have to adapt the infrastructure. We need a new cryogenic system, for example, to cool the cavities far enough for them to become superconducting. Or new bunch diagnostics: with VSR, we will namely have electron packets of different lengths in the ring at the same time. If we are to deliver precisely defined light to the users, we need to know the exact parameters of every single bunch, position-dependently. That takes a lot of effort. As you can see, VSR is a complex project. The basic idea is relatively simple, but the details are quite involved.



In conversation with Hannes Schlender: Prof. Jankowiak is already thinking about BESSY III and his goal is to provide users with high-brilliancy light and flexibly adjustable parameters.

And the users are already lining up?

That may be a little bit of an exaggeration. But, we are in close communication with the scientific community who currently uses BESSY II. And we are discussing with them what they expect from us and what we can deliver. Alexander Föhlisch, head of the institute "Methods and Instrumentation of Research with Synchrotron Radiation" has already discussed the scientific case for BESSY-VSR with the HZB colleagues and the BESSY users. We have gained a lot of valuable knowledge from that, about what is important to the community for the VSR concept. Alexander is the driving force who keeps the user's perspective in the focus of the project. Also, Antje Vollmer, who is responsible for user coordination at BESSY, regularly organises what we call the foresight workshops. With these, she has created a discussion platform for current and potential users to discuss future projects and research activities. The aim is to identify new research fields for BESSY-VSR and to define the requirements for a future BESSY III. A machine like BESSY lives from meeting the expectations of science. The users are showing great interest in these discussions.

And now, with bERLinPro, you are responsible for another major project – are two such ambitious projects not a little too much?

We are more than just working to capacity, there is no question about that. It has always been difficult so far to find the necessary time for bERLinPro. But there are many links between the two projects. In bERLinPro, we are making the prototype of an energy recovery linac, that is a linear accelerator that recovers the energy from the high-energy electron packets after their flight through the beam guidance system. The cavities have to satisfy similar requirements as those for the VSR. The synergies between bERLinPro and VSR are large and, when the workforce expansion for VSR is concluded, will benefit both projects.

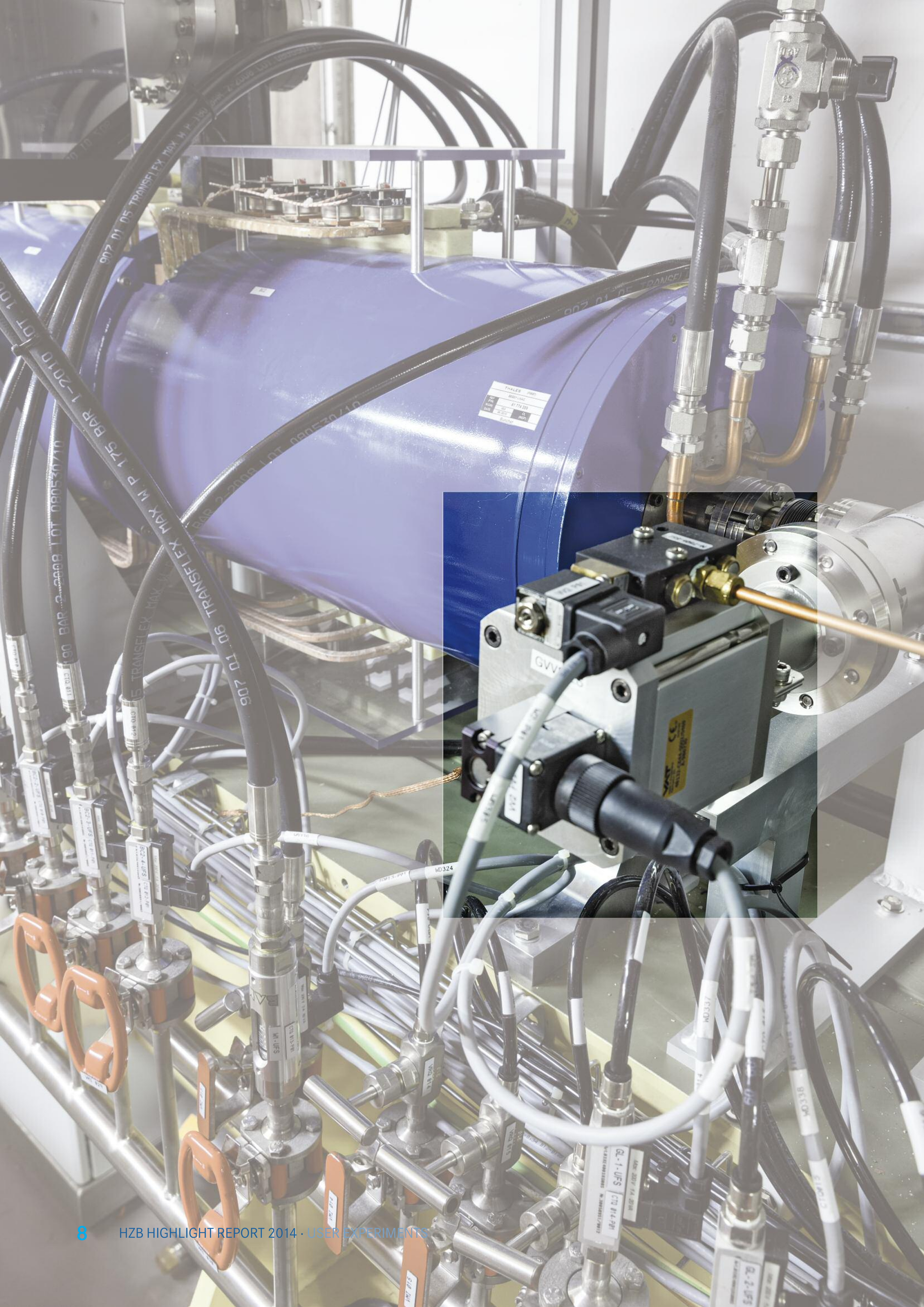
And what comes after BESSY-VSR?

You're referring to BESSY III, and thus far into the future, at least 10 to 15 years. But it is a good question, of course, those being the run-up periods for a large project like a new synchrotron radiation source. At the moment, the sky's the limit. The aim is to provide the user community with the optimal machine. In future, we are still going to stay within our low-energy wavelength range: Soft X-ray radiation is our specific niche, and we want to keep it. And, of course, we want to continue providing many users with high-brilliancy light and flexibly adjustable parameters at the same time. What a concept for BESSY III looks like in detail, we will just have to wait and find out in the years to come. With VSR and bERLinPro, at any rate, we are making important contributions to these deliberations.

Hannes Schlender conducted the interview

SUMMARY

- The synchrotron source BESSY II has run extremely reliably for 15 years. With the BESSY-VSR project, it will be upgraded in future to offer light pulses of different lengths.
- The HZB has already completed and positively assessed the technical design study; funding applications are underway.
- The technical components for realising the project – including the superconducting high-frequency cavities for shortening the electron packets – still need to be developed.
- The HZB is continually exchanging ideas for the project with the scientific community.



HIGHLIGHTS FROM USER EXPERIMENTS

More than 3,400 user visits to the electron storage ring BESSY II in Berlin-Adlershof were recorded in 2014, working in 455 research groups from 30 countries.

298.67 days went into scientific use of the storage ring facility BESSY II in the past year. The scientists had 7,168 operating hours or 896 eight-hour shifts at their disposal. The operational availability equates to 82 percent. 1,040 hours or 130 shifts were used for accelerator experiments. At 26 beamlines and 38 experimental stations, the visiting experimenters had 26 times 766 shifts at their disposal. This added up to a combined figure of 19,916 eight-hour shifts.

4,475 shifts were used for the further development of experimental stations and for preparing the experiments. 1,517.5 shifts were unavailable due to technical reasons, maintenance and training. Factoring in the availability of individual beamlines and experimental stations, a total of 10,895.5 shifts could be used by visiting experimenters and HZB in-house scientists. The 26 beamlines of the storage ring facility BESSY II therefore had an operational availability of 54.7 percent.

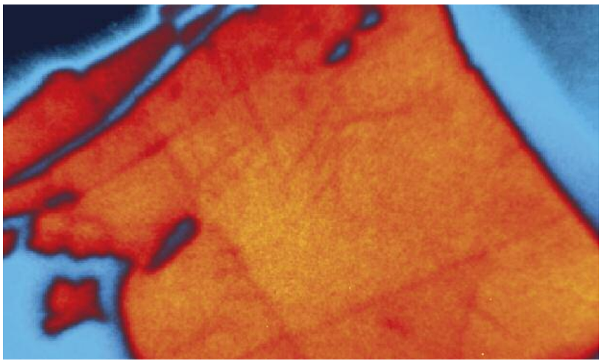
77.7 Prozent or 8,466.5 shifts of the available shifts for scientific research, that were in fact used by scientists, were used for external scientific projects. HZB in-house scientists used 22.3 percent or 2.430 shifts for their own research.

February 2015: After elaborate upgrading and streamlining measures had been carried out during the whole of 2014, the neutron source BER II was put back into operation and made available to the international user community. In spite of the reactor operation being interrupted, measuring time applications for the BER II instrumentation were accepted within the scope of the HZB proposal rounds 2014-II. A total of 128 measuring time applications were submitted and assessed.

STICKY TAPE AND SEMICONDUCTORS

American scientists have discovered a **new class of semiconductors**, and studied their electrical and optical properties at BESSY II. So-called van der Waals' heterostructures could in future deliver new LEDs or lasers.

Painstakingly, the young researcher Hui Fang of the University of California, Berkeley, peels off invisibly thin layers from a material called tungsten selenide; monolayers only one molecule thick. It may not exactly look like doing research on modern high-tech materials, but after long development, it could culminate in new superconductors, light-emitting diodes or lasers. Not that it is surprising she is using this method; after all a similarly fiddly application of sticky tape earned Andrei Geim of the University of Manchester a Nobel Prize in physics in 2010 for the discovery of graphene. Ever since, researchers have turned their attention to substances of comparable structure such as tungsten selenide and molybdenum sulphide. These chalcogenides are the subject of interest for Prof. Ali Javey and colleagues in Berkeley, with whom Hui Fang worked until recently.



The sample consists of a layer of tungsten selenide (orange) applied to a layer of molybdenum sulphide (blue). Studies with the SPEEM microscope at BESSY II show that energy transfers between the two semiconductor layers yields an electric potential of up to 400 meV.

Structural similarities

Tungsten selenide and molybdenum sulphide consist of a plane of positively charged tungsten or molybdenum atoms sandwiched between two laterally offset planes of negatively charged selenium or sulphur atoms. “Such monolayers of a positive and two negatively charged planes hold together very well in-plane,” explains HZB researcher Dr. Florian Kronast. The only bonds to the next three-plane monolayer above or below are so-called van der Waals' attractions which, similarly to graphene, are much weaker than the in-plane forces. These weak bonds above and below can be broken relatively easily, and a piece of adhesive tape is sufficient to lift off one of the three-plane monolayers.

That is exactly what the researchers in Berkeley did, targeting novel materials consisting of such “van der Waals' heterostructures”. Not only are these monolayers semiconductors, but they can also – in theory at least – be stacked on top of one another like Lego bricks. A tungsten selenide layer, for example, could be laid on top of a molybdenum sulphide layer. The new structures are a million times thinner than a sheet of paper and are very stable. This is because considerably stronger interactions take place between the different layers compared to those in the pure substances. Furthermore, the two ultra-thin layers, of only one molecule thickness each, combine to create common properties that neither tungsten selenide nor molybdenum sulphide possesses on its own. For example, electric charges can be exchanged between the two different molec-ule layers. This property is essential for producing LEDs or lasers.

Example of charge exchange

The US researchers in Berkeley, however, were lacking direct evidence of this particular charge exchange. The evidence was delivered by Florian Kronast and colleagues at the HZB. For this, they shone soft X-ray light from the synchrotron BESSY II onto the thousandths-of-a-millimetre-thick double-layers of tungsten selenide and molybdenum sulphide produced in Berkeley. This radiation knocks electrons of different energy states out of the material, which thanks to the SPEEM electron microscope designed specifically for this purpose, can deliver a very accurate picture of the mini-structures. At the same time, the energy filter of the SPEEM resolves the spectrum of the different electron energies.

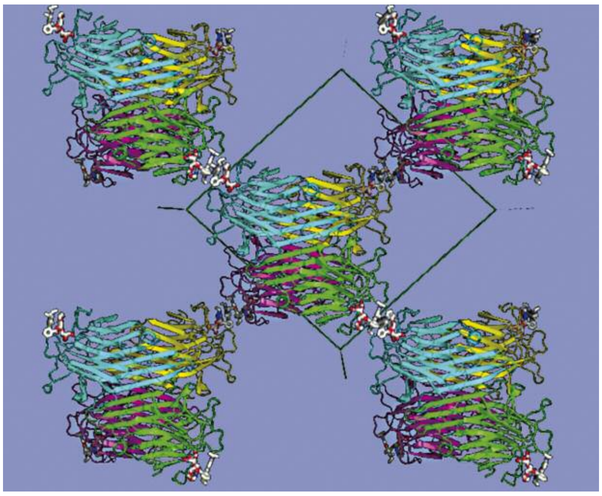
The researchers thus obtain a molybdenum and a tungsten spectrum from the two individual monolayers. Measuring the same spectra on the double-layer reveals a shift in the electron energies. “From this shift in the spectra, you can calculate the charge transfer between the two layers,” Florian Kronast explains. This calculation, in turn, clearly shows that the van der Waals’ heterostructures deliver as promised. Hui Fang’s painstaking manual work has paid off, and the path towards making tailored lasers and light emitting diodes (LEDs) out of these materials is at least theoretically clear. *rk*

PNAS, 111(7), 6198-6202, 2014 (DOI: 10.1073/pnas.1405435111): Strong interlayer coupling in van der Waals’ heterostructures built from single-layer chalcogenides; H. Fang, C. Battaglia, C. Carraro, S. Nemsak, B. Ozdol, J.S. Kang, H.A. Bechtel, S.B. Desai, F. Kronast, A.A. Unal, G. Conti, C. Conlon, G.K. Palsson, M.C. Martin, A.M. Minor, C.S. Fadley, E. Yablonovitch, R. Maboudian and A. Javey

PROTEINS: NEW CLASS OF MATERIALS DISCOVERED

A German-Chinese research team gleans seminal insights into **protein crystalline frameworks** at HZB's BESSY II. This new class of materials consists of proteins that build stable crystals by adding helper molecules.

Proteins are sensitive molecules. Everyone knows that – at least from having boiled eggs. Under certain circumstances – such as immersion in boiling water – they denature, losing their natural shape and becoming hard. True, researchers have been able to handle these substances for some time now, even to the point of crystallizing them in their native state. Although admittedly, this requires considerable effort, it is the only way in which researchers can find out the structure of these substances at high resolution. Moreover, protein crystals are extremely fragile, highly sensitive and hard to handle.
Now, for the first time ever, scientists at China's Fudan University have managed to work around these downsides by linking the protein concanavalin A to helper molecules belonging to the sugar family, and to the dye rhodamin. The concanavalin molecules that have thus been fixated tended to arrange themselves symmetrically within the helper molecule framework, forming crystals in which the proteins achieve high stability and are intricately interconnected – into a protein crystalline framework.



Arrangement of the 237-amino-acid concanavalin A protein molecule (in colour) in a protein crystalline framework (PCF). Helper molecules of the sugar family (red-white) keep the framework stable.

Helper molecules have an impact on protein crystals

Developing molecular structures such as these is pointless unless you know exactly how they form and what their structure looks like at the level of the atoms. During the quest for suitable experimental methods, the Shanghai researchers turned to a Chinese scientist working at the HZB for help. She called her colleagues' attention to the MX beamlines at the HZB's electron storage ring BESSY II.
“Here at the HZB, we were able to offer them our highly specialized crystallography stations – the perfect venue for characterizing PCFs at high resolutions,” says Dr. Manfred Weiss, one of the leading scientists working at the HZB-MX laboratory. It quickly became clear that the helper molecules even allowed the researchers to decide how powerfully they wanted them to penetrate the protein frameworks. “This gives the PCFs a great deal of flexibility and variability, which we’ll always keep in mind when doing research on potential applications,” says Manfred Weiss. *hs*

Nature Communications, 5, 2014, 4634 (DOI: 10.1038/ncomms5634): Protein crystalline frameworks with controllable interpenetration directed by dual supramolecular interactions; F. Sakai, G. Yang, M.S. Weiss, Y. Liu, G. Chen and M. Jiang

ANTIQUE OSIRIS FIGURINES EXAMINED WITH NEUTRONS

An Italian research team used various methods to analyse **three Egyptian bronze figurines** and discover more about their creation. One of the methods was neutron tomography, carried out at the HZB and supervised by Dr. Nikolay Kardjilov.

Historical artefacts are of inestimable value to research because they reveal a great deal about the life and culture of ancient civilizations. The challenge scientists face when studying them, however, is that in most cases they cannot take material samples because doing so would damage the valuable objects. It was no different for the three figurines from the Egyptian Museum in Florence recently studied by Italian researchers. The miniature sculptures embody Osiris, the god of the afterlife, the underworld and the dead, who is a central figure among the Ancient Egyptian gods. The statuettes depict Osiris in a pose typical for the deity, with arms and legs bound, mummy-like, in bandages against the body, the arms crossed over the chest and the two traditional insignia of divine authority held in his hands: the crook and flail. Each figurine also wears the so-called Atef crown, which symbolises sovereignty over Upper and Lower Egypt.

This bronze figurine from the Egyptian Museum in Florence depicts the ancient Egyptian god Osiris. An Italian research team studied the alloy it is made of using neutron tomography at the HZB.

Two methods – one goal

The bronze Osiris figurines are part of the collection of the Egyptian Museum of Florence. One figurine was brought to Italy from the Schiaparelli archaeological expedition at the beginning of the 20th century and is the largest statue, at a height of 37 centimetres and a weight of 1.4 kilograms. The other two statues, only about half the size and significantly lighter, were already donated to the museum by a noble family in 1848 and 1868. The exact origins and ages of the figurines remain unknown.

Juri Agresti, Iacopo Osticioli and Salvatore Siano of the Istituto di Fisica Applicata “Nello Carrara”, Maria Cristina Guidotti of the Soprintendenza per i Beni Archeologici della Toscana and Giuseppina Capriotti of the Istituto di Studi sul Mediterraneo Antico worked together to learn how the figurines were produced and of what materials they are made. They also wanted to explain why the artefacts are in different states of preservation. For the first time, the researchers combined several non-invasive methods to decrypt the mystery of the Osiris figurines’ creation. They employed neutron tomography at the neutron source BER II of the HZB, time-of-flight neutron diffraction at the neutron source ISIS at the Rutherford Appleton Laboratory in the UK, and laser-induced plasma spectroscopy. These three methods each gave the research group different but complementary information about the bronze statuettes.

Three-dimensional images of the inside of each figurine

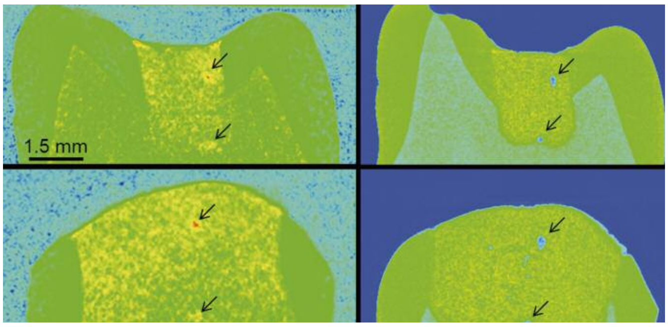
“Neutrons are highly suitable for studying metallic materials. They can penetrate deep into the objects. On our instrument CONRAD at the neutron source BER II, we were able to produce three-dimensional images of the inside of each Osiris figurine,” says Dr. Nikolay Kardjilov, co-author of the paper and responsible scientist for the neutron tomography instrument at the HZB. The analyses showed that all three figurines consist of a similar clay core and that the ancient craftspeople had each used a very similar method to produce the casting moulds for the bronze statuettes. The figurines are also made of metal alloys very similar in composition. This result surprised the scientists, because the figurines appear to have been made in different regions of Egypt. Based on the many insights gained, further bronze statuettes of the Egyptian Museum in Florence will be studied with this promising combination of methods. *SZ*

J. Anal. At. Spectrom., 2015, 30, 713-720; (DOI: 10.1039/C4JA00447G): Combined neutron and laser techniques for technological and compositional investigations of hollow bronze figurines; J. Agresti, I. Osticioli, M. C. Guidotti and G. Capriotti, N. Kardjilov, A. Scherillo and S. Siano

HOW TO PREPARE DURABLE TOOTH CEMENT

An interdisciplinary team of dentists and materials scientists, using **neutron imaging and x-ray-microtomography**, was able to demonstrate how much the order of mixing steps matters to obtain a nearly homogeneous filling without large liquid-filled pores which reduce stability.

Fillings have to resist huge mechanical forces as well as bacteria and chemicals. One of the classics, silver amalgam filling, has the disadvantage of containing mercury, which can poison the environment. And composite materials based on acrylate do not normally last for a lifetime under the harsh conditions in the mouth. An interdisciplinary team of dentists and materials scientists from Niels Bohr Institute at the University of Copenhagen, Denmark, therefore decided to study with glass ionomer cement, a mercury-free filling that has good biological properties, while being almost as strong. “Our research therefore focuses on understanding the connection between the microstructure of the material and its strength in order to improve its properties,” explains Ana Benetti, dentist and researcher at the Faculty of Health and Medical Sciences at the University of Copenhagen. Glass ionomer cement also has the property that when pulverised, it can be mixed with a liquid by hand without the use of special equipment and the material does not need to be illuminated with a lamp to harden (this is necessary for composite materials). This is a great advantage in remote areas without electricity such as in Africa, China or South America.
The researchers studied two kinds of glass ionomer cement. The cement itself is the same, but a mix of acids was blended into one of them. Because of that, two different kinds of liquids were used to mix the cement powder, either ordinary water (for the cement with acids) or water with an acidic mixture (for the cement without acids). The question now was whether it was best to mix the acid with the cement powder or with the water? “It is OK for the material to be porous, however, if the pores contain liquids, it can be a problem since that can make it easier for the fillings to break,” explains Heloisa Bordallo, materials researcher at the University of Copenhagen. To find out, they contacted Nikolay Kardjilov and Ingo Manke at the neutron source BER II at Helmholtz-Zentrum Berlin, who are experts in 3D imaging with neutrons and X-rays.
“Our neutron tomography instrument CONRAD II provides the highest spatial resolution worldwide, comparable to the resolution of the micro-CT with X-rays, which we can do in the lab next door”, Kardjilov explains. First they took X-rays of different teeth with the cement fillings to get an accurate image in 3D of the microstructure, showing location and size of the pores. The neutron tomography allowed them to detect the presence of hydrogen atoms and liquids inside the pores and in the material.



The neutron images (left row) detect the distribution of liquids in this filled tooth, whereas the X-ray-CT shows the microstructure and pores in the material. A comparision of both images shows which pores are filled with liquids.

Strongest materials with “acidic” water

The results show that the “easiest way” of preparation with ordinary water is not the best: when the cement is already mixed with acids and just ordinary water remains to be added, the material is weakest. “We get the strongest material by having cement powder mixed with water that has had acid added to it. So it is better to have the acid in the water – it helps to bind the liquid faster and stronger to the cement and there is less water in the pores,” explains Heloisa Bordallo. There is still too much loose liquid in the pores, so now the research is continuing with new mixtures where they will try adding natural minerals to the cement.

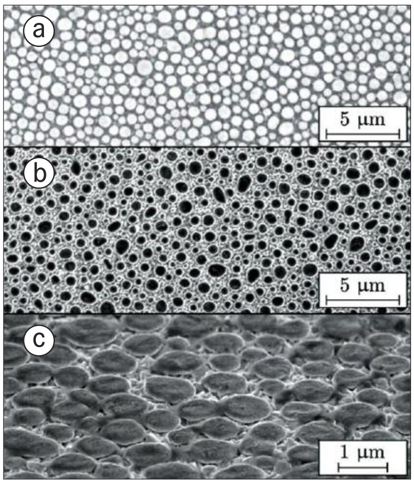
arö/Uni Copenhagen

Scientific Reports, 5, 8972 (DOI:10.1038/srep08972): How mobile are protons in the structure of dental glass ionomer cements?; A.R. Benetti, J. Jacobsen, B. Lehnhoff, N.C.R. Momsen, D.V. Okhrimenko, M.T.F. Telling, N. Kardjilov, M. Strobl, T. Seydel, I. Manke and H.N. Bordallo

COLLECTING LIGHT WITH ARTIFICIAL MOTH EYES

Scientists at Eidgenössische Materialprüfungs- und Forschungsanstalt (EMPA) and University of Basel have analysed a **photoelectronic cell** at BESSY II, recreating a moth's eye to drastically increase its light collecting efficiency.

Rust – iron oxide – could revolutionise solar cell technology. This usually unwanted substance can be used to make photoelectrodes which split water and generate hydrogen. Sunlight is thereby directly converted into valuable fuel rather than first being used to generate electricity. Unfortunately, as a raw material iron oxide has its limitations. Although it is unbelievably cheap and absorbs light in exactly the wavelength region where the sun emits the most energy, it conducts electricity very poorly and must therefore be used in the form of an extremely thin film in order for the water splitting technique to work. The disadvantage of this is that these thin-films absorb too little of the sunlight shining on the cell. EMPA researchers Florent Boudoire and Dr. Artur Braun have now succeeded in solving this problem. A special microstructure on the photoelectrode surface literally gathers in sunlight and does not let it out again. The basis for this innovative structure are tiny particles of tungsten oxide which, because of their saturated yellow colour, can also be used for photoelectrodes. The yellow microspheres are applied to an electrode and then covered with an extremely thin nanoscale layer of iron oxide. When external light falls on the particle it is reflected internally back and forth, until finally all the light is absorbed. All the entire energy in the beam is now available to use for splitting the water molecules.



Ammonium tungstate/PSS film surface: (a) SEM image before pyrolysis; (b & c) SEM image after pyrolysis.

"In principle the newly conceived microstructure functions like the eye of a moth," explains Florent Boudoire. "The eyes of these night-active creatures need to collect as much light as possible to see in the dark, and must also reflect as little as possible to avoid detection and being eaten by their enemies. The microstructure of their eyes is especially adapted to the appropriate wavelength of light. EMPA's photocells take advantage of the same effect."

"Capturing light" simulated on the computer

In order to recreate artificial moth eyes from metal oxide microspheres, Boudoire sprays a sheet of glass with a suspension of plastic particles, each of which contains at its centre a drop of tungsten salt solution. The particles lie on the glass like a layer of marbles packed close to each other. The sheet is placed in an oven and heated, the plastic material burns away and each drop of salt solution is transformed into the required tungsten oxide microsphere. The next step is to spray the new structure with an iron salt solution and once again heat it in an oven.

Now, one could interpret these mixing, spraying and burning processes as pure alchemy – a series of steps that is eventually successful by pure chance. However, in parallel to their practical experiments, the researchers have been running calculations modelling the process on their computers and have thus been able to simulate the "capturing of light" in the tiny spheres. "The results of the simulation agree with the experimental observations," as project leader Artur Braun confirms. The Swiss team analysed their samples under the X-ray microscope at BESSY II in order to get detailed information about the absorption of light and the chemical processes which enhance it. It is clear to see how much the tungsten oxide contributes to the photo current and how much is due to the iron oxide. Also, the smaller the microspheres, the more light which lands on the iron oxide underneath the tiny balls. As a next step, the researchers plan to investigate what the effect of several layers of microspheres lying on top of each other might be. The work on moth eye solar cells is still in progress! *EMPA/arö*

Energy Environ. Sci., 2014,7, 2680-2688 (DOI: 10.1039/C4EE00380B): Photonic light trapping in self-organized all-oxide microspheroids impacts photoelectrochemical water splitting; F. Boudoire et. al.

MESSAGES FROM SPACE

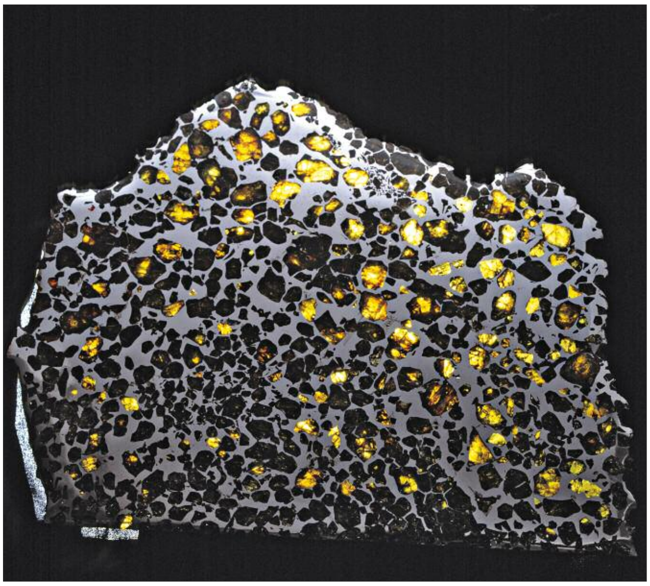
Geologists from the University of Cambridge have uncovered hidden **magnetic messages from the early solar system in meteorites** measured at BESSY II. They could provide a sneak preview of the fate of Earth's own magnetic field.

Meteorites have witnessed a long and violent history; they are fragments of asteroids which formed in the early solar system, 4.5 billion years ago. Shortly after their formation, some asteroids were heated up by radioactive decay, causing them to melt and segregate into a liquid metal core surrounded by a solid rocky mantle. Convection of the liquid metal created magnetic fields, just as the liquid outer core of the Earth generates a magnetic field today. "Meteorites are like natural hard discs", Dr. Richard Harrison believes. The geologist from the Department of Earth Sciences, University of Cambridge, UK, is searching for methods to decipher the information stored deep inside the space rocks.

Particles of tetrataenite reveal early magnetic fields

At the PEEM-Beamline of BESSY II, Harrison and PhD student James Bryson found dramatic variation in magnetic properties as they went through the meteorite. They saw not only regions containing large, mobile magnetic domains that can easily be overwritten, but also identified an unusual region called the cloudy zone containing thousands of tiny particles of tetrataenite, a super-hard magnetic material. "These tiny particles, just 50 to 100 nanometres in diameter, hold on to their magnetic signal and don't change. So it is only these very small regions of chaotic-looking magnetization that contain the information we want", Bryson concludes.

The PEEM-Beamline offers X-rays with the specific energy and polarization needed to make sense of these magnetic signals. Since the absorption of the X-rays depends on the magnetization, the scientists could map the magnetic signals on the sample surface in ultrahigh resolution without changing them by the procedure. "The new technique we have developed is a way of analysing these images to extract real information. So for the first time, we can conduct paleomagnetic measurements on very small regions of these rocks, regions which are less than one micrometre in size. These are the highest-resolution paleomagnetic measurements ever made", Harrison points out. By spatially resolving the variations in magnetic signal across the cloudy zone, the team was able to reconstruct the history of magnetic activity on the meteorite parent body, and were even able to capture the moment when the core finished solidifying and the magnetic field shut down. These new measurements answer many open questions regarding the longevity and stability of magnetic activity on small bodies. Their observations, supported by computer simulations, demonstrate that the magnetic field was created by compositional, rather than thermal, convection – a result that changes our perspective on the way magnetic fields were generated during the early solar system and even provides a sneak preview of the fate of Earth's own magnetic field as its core continues to freeze. *arö*



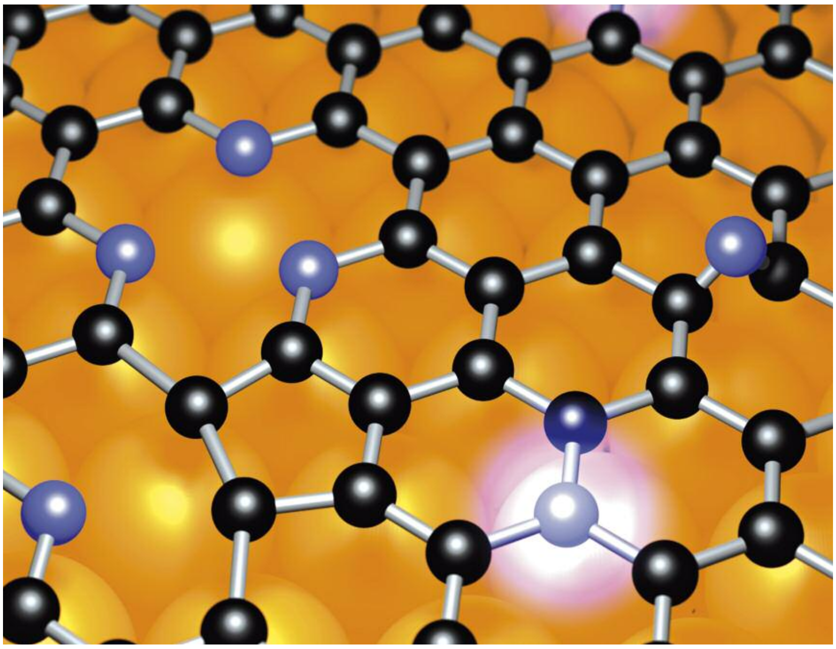
Hard disc from space: the Pallasite meteorite, studied by Harrison, contains information about the early solar system.

Nature, 517, 2015, 472–475 (DOI: 10.1038/nature14114): Long-lived magnetism from solidification-driven convection on the pallasite parent body; J.F.J. Bryson, C.I.O. Nichols, J. Herrero-Albillos, F. Kronast, T. Kasama, H. Alimadadi, G. van der Laan, F. Nimmo and R.J. Harrison

FITNESS PROGRAMME FOR GRAPHENE

A German-Russian research team has **combined graphene with nitrogen, as well as with cobalt and nickel**. Their aim is to modify graphene to make it suitable for practical use in technologies such as batteries and spintronic processors.

When two Russian physicists, Andre Geim and Konstantin Novoselov, first reported the production of graphene flakes and demonstrated its astonishing properties, there was intense enthusiasm and interest within the research community. Alongside graphite, diamond, nanotubes, and fullerenes, graphene is a formation of carbon and was rapidly recognized as a hot candidate for diverse technological applications. In this "wonder material", the carbon atoms are linked together to form a honeycomb structure: six atoms in each case create a ring, which constitutes a mesh together with its neighbouring rings. The mesh is only one single atomic diameter thin and has plenty of exceptional characteristics: the material is chemically inert and mechanically extremely stiff, very flexible and has a high electrical and thermal conductivity. Researchers hope that innovative graphene forms can be turned into sensors, nano-electrical elements – or that components for future quantum computers and highly efficient batteries can be built.


Graphene populated with different nitrogen impurities (blue atoms). The underlying gold surface promotes the controllable conversion of impurity-related defects into substitutions (glowing atoms), which effectively donate electrons to N-graphene.

Yet challenges in production remain to be overcome for graphene to play a role in such exciting applications and technologies. As a so-called zero-gap semiconductor, pure graphene does not appear ready for direct implementation in electronic devices. Therefore, many research efforts are directed towards the elaboration of methods to both induce and fine-tune a semiconducting gap in graphene. To create and control the semiconducting properties of pristine graphene, doping is regarded as one of the most feasible methods. A group of researchers from Saint-Petersburg and Dresden Universities led by Dr. Dmitry Usachov and Dr. Denis Vyalikh has recently presented an approach that allows the incorporation of atoms of nitrogen (N) or boron (B) into the graphene's mesh. Their experimental expertise combined with computational methods has allowed the creation of two-dimensional systems that are called N- and B-graphene as well as conclusively exploring the unique electronic and structural properties of these materials.

Targeted control over nitrogen imperfections

It is anticipated that graphene modified in this way might be a suitable material for use in batteries, supercapacitors, fuel cells and a myriad of other electronic and chemical applications. For example, to make N-graphene samples on metallic substrates, the researchers have suggested using a chemical vapour deposition approach, where as a precursor s-triazine molecules are utilized. S-triazine is an organic compound including nitrogen atoms. Each of them contains one additional electron, and thus upon replacing a carbon atom in the graphene lattice, novel electronic properties of the resulting system can be envisaged. It is known that incorporation of nitrogen atoms into the carbon matrix can lead to the appearance of different kinds of impurities. The joint team of researchers has discovered an approach allowing precise control over the nitrogen's incorporation into the graphene matrix, which efficiently converts the defect-like N impurities into the graphitic configuration. The latter is highly important for the desired electron doping effect, and for tuning the band structure and carrier concentration of N-graphene.

On the path to the spintronics processor

In addition to N- and B-doped graphene, the researchers also have another application for this exotic material in mind: as a basic material for the development of spintronics. This new generation of electronics is not only based on the currently standard method of controlling the charge of electrons – it also utilizes its spin. The latter can be regarded as the angular momentum of an electron, and it can be manipulated with magnetic fields. It is believed that one can further use the spin of an electron together with its charge for logic and data storage applications.
The development of spintronics is still in its nascent stages. One challenge that remains open is finding systems able to produce spin current with well-defined properties. The researchers from Dresden and Saint-Petersburg favour graphene for this use, combined with a ferromagnetic layer of ferromagnetic cobalt. If grown on a single crystalline layer of ferromagnetic cobalt under appropriate conditions, graphene becomes precisely oriented with the metallic substrate. This combined system exhibits a highly mobile two-dimensional gas of spin-polarized charge carriers. Compelling evidence was shown demonstrating how the graphene/cobalt interface becomes a very intriguing and promising system for spintronic applications. Last but not least, all these results have been achieved due to the recently developed instrumentation at BESSY-II. The latter has been developed by the same groups of researchers, in very close cooperation with the staff members of the HZB.

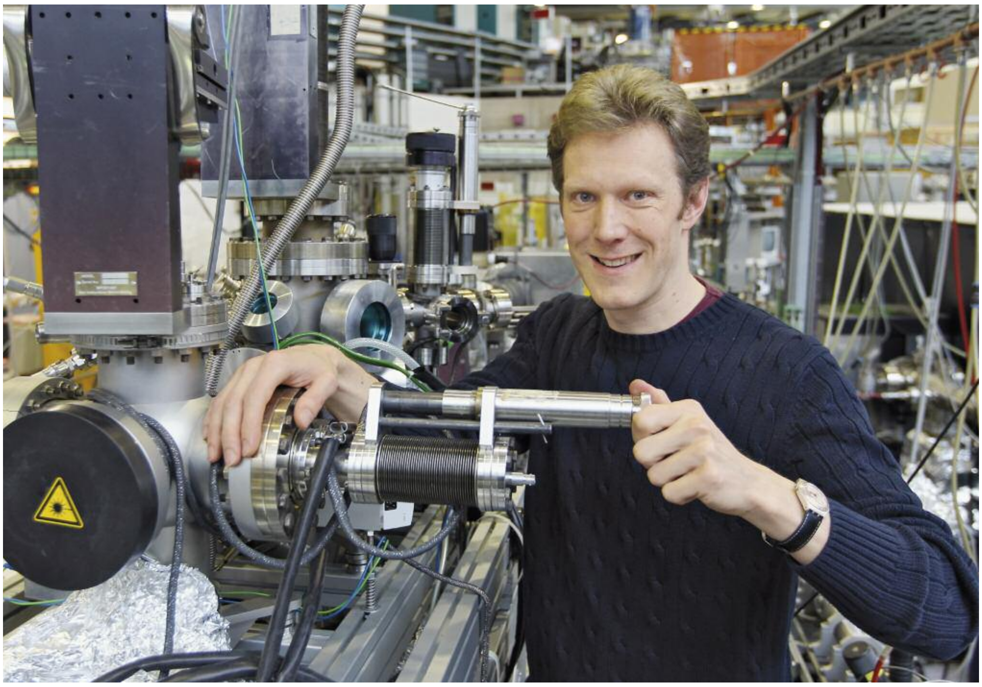
rb

Nano Lett., 2014, 14 (9), pp 4982–4988 (DOI: 10.1021/nl501389h): The chemistry of imperfections in N-graphene; D. Usachov et. al.

O ANGULAR MOMENTUM, WHERE ART THOU?

French scientists and colleagues from the HZB have studied the **angular momenta of two different ferrimagnets** under the influence of laser beams. The ability to control momentum transfer processes on a microscopic scale and in femtosecond timeframes is the key to ultra-fast data storage.

Ferrimagnets are odd materials: they contain different regions of opposing magnetic order. This ordering arises due to the orbital motion of electrons and their spins – which is a kind of intrinsic angular momentum of the particles. Since the magnetisation of the crystalline regions can be of different strengths, many ferrimagnets – typically metal alloys – exhibit net magnetism on the whole. Even if their inner structure is not fully understood, this makes the materials candidates for developing novel magnetic data storage devices that can record gigantic volumes of data, and read and write them at very high speed. Such storage devices would exploit the angular momentum of the material, which is intimately connected with its magnetisation and can be switched for storing data. With ever-increasing miniaturisation, the ferromagnetic materials so far used are reaching a limit at which thermal instability of the bits is leading to loss of stored information.
"Before any technical use, it is necessary to understand what goes on inside the materials at the microscopic level," says physicist Dr. Christian Stamm. One question that has remained open until recently is: how is angular momentum conserved, say, when laser light is shone onto a magnetic material to store or delete data? Stamm, who researches in the Magnetism and Interface Physics group at the Swiss Federal Institute of Technology (ETH) Zürich and who previously worked for nine years at HZB, has now managed to



Dr. Christian Stamm, who formerly worked at HZB, once again used the worldwide unique possibilities of the femtosecond source at BESSY II for his research on angular momentum transfer processes.

answer this question together with research colleagues from the French Universities of Strasbourg and Nancy and colleagues from the HZB. For their experiments, the team chose two different ferrimagnetic alloys: one made of cobalt and gadolinium and the other of cobalt and terbium. The researchers studied these using X-ray laser light pulses from one of the femtosecond sources at the synchrotron storage ring BESSY II of the HZB.

Fast transfer of angular momentum

There, they fire laser pulses a few femtoseconds (trillionths of a second) in duration at electrons flying through the ring at almost light speed, which subsequently emit X-ray light. Given the rhythm of the laser pulses, an ultrafast temporal structure is obtained: this results in femtosecond-short, strobe-like X-ray flashes by which the materials can be seen through. A remarkable feature is that the flashes are not only extremely short, but are also circularly polarised, and are therefore ideal for studying magnetism. "This is unique in the world," Stamm enthuses. "Besides the HZB, there is no other source that offers these experimental conditions."
The combination of X-ray light and circular polarisation is the decisive factor. It allows you to look deep into the heart of the material and follow ultrafast processes – even selectively for the different chemical elements in the sample.
The method is called magnetic circular dichroism spectroscopy. With this method, Stamm and his team have succeeded for the first time in observing, at extremely precise temporal resolution, how the angular momenta in the two ferrimagnetic alloys behave after excitation by laser pulse.
The researchers' results show that the alloy of cobalt and gadolinium, in which the magnetisation of the two crystalline sublattices mutually cancel each other out, still possess a net angular momentum of zero even after excitation. So, from the outside, it looks like nothing changes. But inside the crystal, fundamental and very fast changes take place: "The spins in the two sublattices lose their alignment due to the laser pulse; their magnetic order is lost," Stamm explains. "Apparently, angular momentum is transferred between cobalt and gadolinium." And that takes place within about a hundred femtoseconds.

Puzzling angular momentum transfer in terbium

The behaviour inside the terbium-containing alloy is different: in the initial state, terbium has a larger angular momentum than cobalt, yielding a non-zero net angular momentum. "Upon laser excitation, only some of the inner order is lost," Stamm says. This actually causes the net angular momentum to almost vanish. "This is an indication that – unlike in the gadolinium-containing alloy – an external reservoir is involved that absorbs the angular momentum," the physicist explains. Another indication that this might be so which the scientists observed is a delay of about 140 femtoseconds during the angular momentum transfer. Exactly where the angular momentum is transferred to is still unknown. Subsequent experiments could bring this to light.
The experiments have yielded valuable new insights: the results of the measurements at the HZB deliver crucial pieces to the puzzle of magnetic materials and the complex physical processes taking place within them. Thus, they help to prepare the materials for their possible use in novel, high-performance and ultrafast data storage devices.

rb

Nature Communications 5, 3466 (DOI: 10.1038/ncomms4466): Ultrafast angular momentum transfer in multisublattice ferrimagnets;
N. Bergeard, V. López-Flores, V. Halté, M. Hehn, C. Stamm, N. Pontius, E. Beaurepaire and C. Boeglin

BRIDGES IN SHAMPOO

The saponin obtained from the soap bark tree is used as an emulsifier in washing detergents and foods. To test it for possible side-effects, Polish researchers used **neutron reflectometry** at the HZB to study its behaviour in contact with biological membranes.

To look at, the soap bark tree *Quillaja saponaria* in the mountain forests of Central Chile seems quite harmless. But the tree certainly knows how to protect its own hide, in that it stores large amounts of saponins in its bark, which defend it against attack from insects. Saponins are natural foam-forming substances and are therefore a subject of great interest to scientists in the cosmetics and food industries, given their broad application potential. The catch: some saponins can break apart red blood cells.
Saponins are found widely throughout the plant kingdom, including in vegetables such as asparagus, tomatoes and potatoes. Because their structures are highly diverse, it is impossible to make a general prediction of how they will affect humans. To avoid nasty surprises, it is best to know the exact properties of each biomolecule in question. It is for this very purpose that researchers such as Dr. Kamil Wojciechowski of the Technische Universität in Warsaw seek the assistance of Dr. Thomas Gutberlet and Dr. Marcus Trapp of the HZB. Alongside their own research, these two scientists supervise the guests who come to the HZB's large research facilities to analyse their samples.
Saponins such as those Wojciechowski is studying from the soap bark tree comprise two distinct halves: one half belongs to a group of substances called terpenoids, which is highly compatible with fats and oils, and the other half is a sugar chain, which interacts well with water. Such an amphipathic molecule can form a bridge between two substances that would otherwise never mix: oil and water. Mayonnaise and ketchup are just such mixtures. Cleansing agents such as shampoos also benefit from this effect, since the terpenoid end holds onto fatty dirt while the sugar end bonds with the washing water, and the dirt is accordingly washed away.

Danger for red blood cells?

To make a better estimate of these emulsifiers' risk to humans, Wojciechowski and colleagues have studied how saponins from the soap bark tree interact with the outer envelope of red blood cells. "Some saponins seem to damage this cell membrane in particular," Thomas Gutberlet explains. How this happens, however, is still largely a mystery. "That is why we are studying the behaviour of these natural substances at the HZB."
To do so, they employed neutron reflectometry at the HZB: similarly to lighting a surface with a light beam, the researchers shone a neutron beam from the neutron source BER II onto the saponins and an artificial membrane that closely resembles the outer wall of a red blood cell. In conjunction with infrared spectroscopy, the reflected neutrons revealed that the saponins do not destroy the membrane, but instead penetrate it and even strengthen it. "Of course that does not mean that saponins in general are harmless to blood cells," the chemist Thomas Gutberlet stresses. After all, there are very many different saponins, and for a structure different than that studied, the results could be quite different. The saponin researchers therefore have much work ahead of them. *rk*

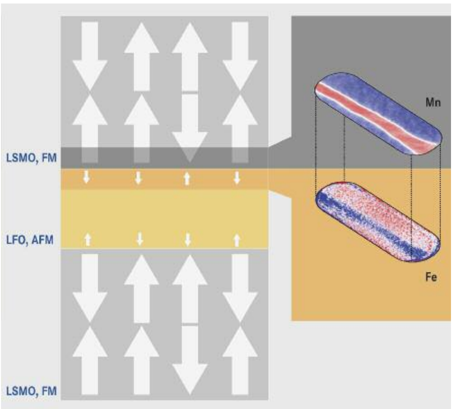
The saponins of the soap bark tree protect the tree against hungry insects. A Polish research group studied at the HZB whether they actually destroy red blood cells.

Biochimica et Biophysica Acta BBA) – Biomembranes, Vol. 1838, Is. 7, pp. 1931-1940 (DOI: 10.1016/j.bbamem.2014.04.008): Unusual penetration of phospholipid mono- and bilayers by Quillaja bark saponin biosurfactant; K. Wojciechowski et. al.

INSIGHT INTO INNER MAGNETIC LAYERS

With measurements at BESSY II an international team of researchers was able to show how spin filters forming within **magnetic sandwiches influence tunnel magnetoresistance**. Their results can help in designing spintronic components.

Layers of magnetic materials are found in every hard drive and in every read/write head today. These are sandwiches made of complex heterostructures in which the different layers have typical thicknesses of only a few nanometres. An effect of quantum physics called tunnel magnetoresistance (TMR) is critical for their operation. It occurs when two ferromagnetic layers are separated from one another by an insulating layer several plies of atoms thick, like cheese between two slices of bread. As long as the magnetisation in both "slices" is parallel, the electrons can tunnel through the "cheese", i.e. the device resistance is low. However, if the magnetisation changes in one of the layers, the electrons can no longer tunnel through the middle layer, i.e. the resistance is high. In this way, the electrical resistance can be precisely controlled through the influence of a magnetic field on one of the two outer layers, and be associated with the binary values of zero and one used for calculations.



The insulating LFO-layer in its normal state is antiferromagnetically ordered (AFM) and has no ferromagnetic domains. Due to the proximity to the ferromagnetic LSMO, ferromagnetic domains develop (white arrows) at the interface, pointing into the opposite direction of the LSMO-layer.

New effect observed

The teams from France, Spain and HZB have discovered that in such sandwiches combining different transition metal oxides, new interfacial effects can strongly influence the amplitude of the TMR. This is what the French team under Manuel Bibes and Agnès Barthélémy of the Unité de Physique, CNRS/Thales, Palaiseau (working in collaboration with the team of Prof. Jacobo Santamaria in Madrid) had initially observed in measuring the electron transport characteristics. They were researching a system of two LSMO ($La_{0.7}Sr_{0.3}MnO_3$), layers that were separated by a very thin layer of LFO ($LaFeO_3$).The LSMO layers were ferromagnetic while the LFO insulating layer was anti-ferromagnetic.

New magnetic order at the interface

Measurements using the ALICE chamber and from the XPEEM instrument in beamline UE49 at BESSY II have clearly shown what is happening in the interface between the ferromagnetic layers and the anti-ferromagnetic inner layer. The teams were able to decode how each of the magnetic elements manganese and iron were oriented at the interfaces using the XPEEM instrument. "We saw how new magnetic phases arise at the boundaries that function like spin filters", explains Dr. Sergio Valencia, who heads the HZB team. "Put simply: the iron atoms near the interface are influenced by the manganese magnetic moments; they then orient their magnetic moments antiparallel to those of the manganese atoms and thus form ferromagnetic domains. We have thus demonstrated experimentally for the first time that ferromagnetic domains can be induced in non-ferromagnetic barrier layers."

The French team carried out subsequent calculations of how these kinds of spin filters affect the tunnel magnetoresistance and could reproduce the experimental data. "These kinds of complex oxide heterostructures as we investigated here could play an important role in future spintronics", says Valencia. The results explain an important process that has not been taken into account so far, and they therefore help in designing tunnel barriers with the desired properties. *arö*

Nature Communications, 6, 6306, (DOI: 10.1038/ncomms7306): Insight into spin transport in oxide heterostructures from interface-resolved magnetic mapping; F. Y. Bruno, M. N. Grisolia, C. Visani, S. Valencia, M. Varela, R. Abrudan, J. Tornos, A. Rivera-Calzada, A. A. Ünal, S. J. Pennycook, Z. Sefrioui, C. Leon, J. E. Villegas, J. Santamaria, A. Barthélémy and M. Bibes

SPINTRONICS: DANCE OF THE NANOVORTICES

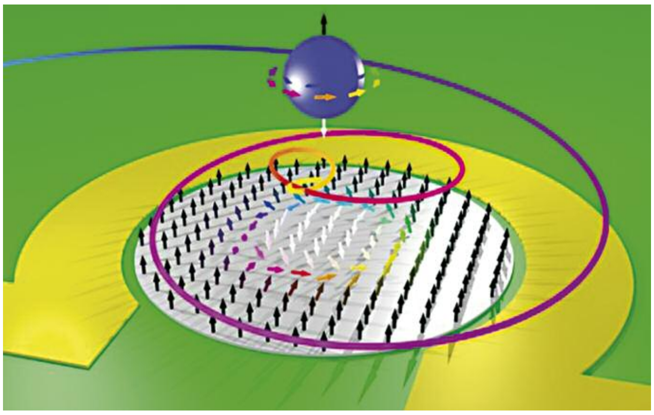
The trajectories of **small magnetic entities** referred to as skyrmions have been captured and recorded with the help of X-ray holography. Researchers suspect that with the help of these skyrmions, units of information can be stored more densely and transferred more reliably than at present.

It is a familiar phenomenon: if a spinning top is bumped or is set in rotation on an inclined surface, it usually does not move in a straight line, but instead describes a series of small arches. Researchers at TU Berlin and the Johannes Gutenberg University Mainz (JGU) together with research teams from the Netherlands and Switzerland have now succeeded in capturing and recording this pattern of movement in a magnetic thin-film system – in the form of small magnetic nanovortices. "With the help of magnetic fields, we can selectively create the magnetic nanovortices, then give them a shove so that they are deflected out of their equilibrium position", explains Dr. Felix Büttner, who pursued this research as his Ph.D. project. "We were then able to very precisely track how these skyrmions, as these special nanovortices are called, return to their rest position", Büttner explains further. The vortices are formed in a magnetic system of thin-film multilayers, where alternating layers composed of a cobalt-boron alloy and platinum are stacked on one another. Each individual layer is less than one nanometre thick, enabling the skyrmions to exist. The diameter of these magnetic vortices is no more than 100 nanometres.

X-ray holography at BESSY II

Special techniques enabled the researchers to track the movements of the skyrmions with a precision of better than a few nanometres at individual time steps less than one nanosecond apart. This was facilitated by holographic recording techniques using intense X-ray pulses of the BESSY II synchrotron source at HZB. These holographic recording techniques have been developed and improved by the TU Berlin "Nanometre Optics and X-ray Scattering" research group in conjunction with HZB over a number of years, a joint effort directed by Prof. Stefan Eisebitt from TU Berlin. What Büttner and his co-workers observed in the X-ray holograms was remarkable: "Similar to bumping a spinning top, the nanovortex does not move in a straight line, but instead along a spiral trajectory", explains Büttner. "By comparing our measurements with model calculations, we were able to determine that this spiral-shaped movement can only be explained if the skyrmion has mass."

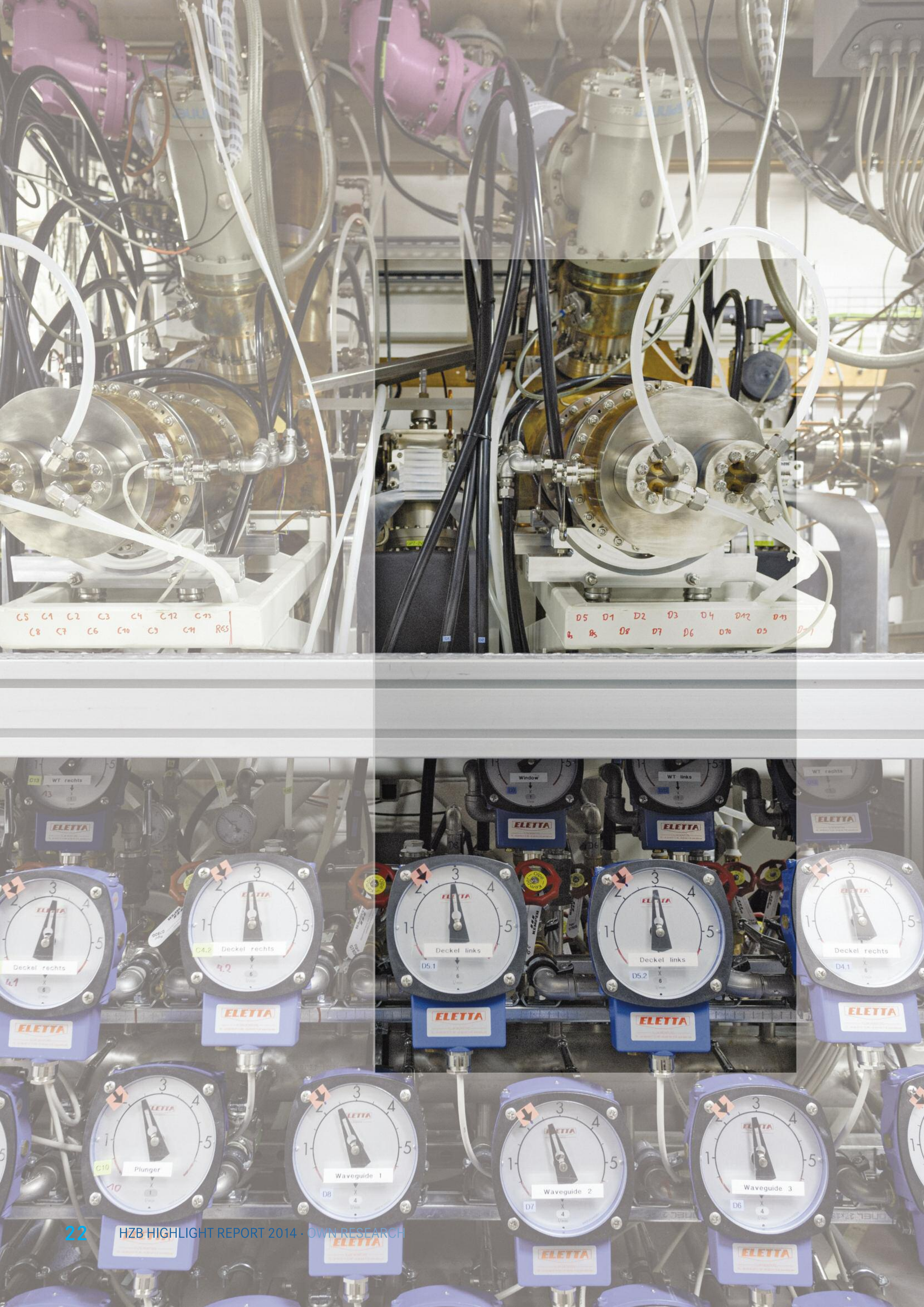
This is an important discovery, since the nanovortices observed here represent only one special type of skyrmion. "In the past, skyrmions were often described as being massless", explains Christoforos Moutafis from the Paul Scherrer Institute, who has long been involved with these kinds of structures. Now, the application of the concept of mass to such particles, as established by this work, will also contribute to the understanding of other types of skyrmions.



The local magnetisation is depicted by small arrows; a magnetic vortex is located in the centre. A brief current pulse through this nano-wire deflects the skyrmion out of its rest position; it then moves back to its initial position on a spiral trajectory. This motion can be observed with the help of X-ray holography. The skyrmion and the spiral shape of its trajectory are represented schematically above the structure.

There could also be tangible applications for these magnetic nanovortices within thin magnetic layers – they are already being discussed today as an alternative information medium in data processing and storage. Researchers suspect that due to their "skyrmion property", such bits (units of information) can be stored more densely and transferred more reliably than at present. The new insights into skyrmion behaviour might contribute to realising these kinds of novel concepts for information processing. *arö*

Nature Physics, 11, 225–228 (DOI:10.1038/nphys3234): Dynamics and inertia of skyrmionic spin structures; F. Büttner et. al.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HIGHLIGHTS FROM OUR OWN RESEARCH

1,160 employees were employed at Helmholtz-Zentrum Berlin für Materialien und Energie in 2014, including trainees. 20 new training contracts were concluded; at the end of 2014 there were a total of 53 young adults working in 10 trained professions at HZB. 322 women were employed at HZB, equating to around 27.8 percent of all employees.

537 ISI-cited papers were published by scientists at HZB in 2014. On top of these were 58 lectured publications. In total, 202 papers were from the field of renewable energies and 393 papers from photon, neutron and ion (PNI) research.

134 postgraduate students were supervised by HZB in 2014. In total, 21 doctoral theses, 4 diploma theses, 35 master theses, 12 bachelor theses and 1 student research paper were concluded. 69 postgrads worked in the field of renewable energies for their thesis and 65 in the field of PNI.

85 joint ventures with companies were entered into by HZB in 2014. The total number of ongoing joint ventures with industry at the end of 2014 was 146 – of these, 61 in the field of renewable energies and 85 in the field of PNI.

8 patents were awarded to the HZB by the German Patent and Trade Mark Office in 2014, of which 4 were in the field of renewable energies and 4 in the field of PNI. At the end of 2014, HZB's patent portfolio encompassed 286 national and international property rights. 42 property rights were objects of ongoing licence agreements.

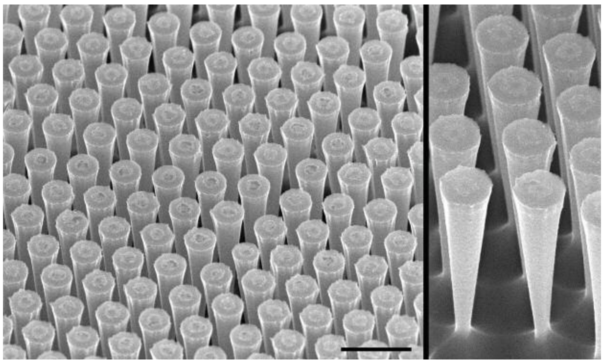
COPIED FROM THE EYE

A **biological structure in mammalian eyes** has inspired a team headed by Prof. Dr. Silke Christiansen to design an inorganic counterpart for use in solar cells: silicon micro-funnels increase the efficiency of solar cells.

The human eye is a fascinating and highly complex sensory organ. With the macula lutea, or yellow spot, it features a discrete area at the very centre of which is the *fovea centralis*. This small area, around 1.5 millimetres in diameter, has the highest density of cones. These slender, conical colour photoreceptors are arranged into a regular mosaic. Because each cone is also directly connected to its own nerve cell, the highest visual acuity is achieved here, meaning we see the sharpest image in this tiny region. This closely packed arrangement of cones has now inspired the team headed by Prof. Silke Christiansen to replicate something similar in silicon as a surface for solar cells and investigate its suitability for collecting and conducting light. Christiansen heads the Institute for Nanoarchitectures for Energy Conversion at the HZB and a research team at the Max Planck Institute for the Science of Light (MPL). "We've shown in this work that the light funnels absorb considerably more light than other optical architectures tested over the last while," says Sebastian Schmitt, one of the two first authors of the publication.

Small change – large effect

Manufacturing the light funnels requires no special effort and is feasible with conventional semiconductor processes such as reactive ion etching or wet chemical etching, for example. In this manner the scientists etched micron-sized vertical funnels shoulder-to-shoulder in a silicon substrate. Using mathematical models and experiments, they tested how these kinds of funnel arrays collect incident light and conduct it to the active layer of a silicon solar cell.
The researchers were surprised at just how large the effect of this architecture was, however. It was known from previous studies that arrangements of very thin vertical cylinders (a "carpet" of silicon nanowires) absorb light well. But even tiny changes from a cylindrical to a funnel shape already increased absorption. Compared to the carpet of nanowires, which has been investigated for some time, the micro-funnels increase photo absorption by about 65 percent and and improve other solar cell parameters as well.



Scanning electron micrographs (SEM) show how regularly the funnels etched in a silicon substrate are arranged (left: the line segment = 5 microns; right: 1 micron). The funnels measure about 800 nanometres in diameter above and taper down to about a hundred nanometres at the tip.

With their modelling, the researchers were also able to explain why the arrays of light funnels trap light considerably better than a carpet of nanowires. Optical modes in nanowires mutually interfere with each other. "A field of closely arrayed nanowires therefore takes in light less efficiently than an identical number of single nanowires could. Just the opposite occurs with the light funnels: immediately neighbouring light funnels mutually strengthen one another's absorption," explains Sebastian Schmitt. "Following this interesting initial result, we are pressing ahead in various directions," says Christiansen. She and her team are working further on improving thin-film solar cells based on silicon and want to build the funnels into robust cell designs that can be economically realised over large surfaces. arö

Scientific Reports, 5, 8570 (DOI:10.1038/srep08570): Enhanced photovoltaics inspired by the fovea centralis; G. Shalev, S.W. Schmitt, H. Embrechts, G. Brönstrup and S. Christiansen and Nano Energy, Vol. 12, 2015, 801-809 (DOI: 10.1016/j.nanoen.2015. 01.048): Maximizing the ultimate absorption efficiency of vertically-aligned semiconductor nanowire arrays with wires of a low absorption cross-section; G. Shalev, S.W. Schmitt, G. Brönstrup and S. Christiansen

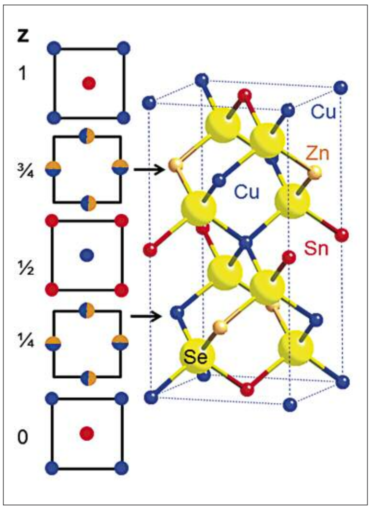
COPPER, TIN AND ZINC FOR SOLAR POWER

In the group of Prof. Susan Schorr, head of the Crystallography department, Dr. Galina Gurieva studied new materials for producing **efficient thin-film solar cells**. These could replace the currently used rare earths, which are expensive and of limited availability.

For producing electric current in thin-film solar cells, the absorber layer is the critical element. It is usually only a few micrometres thick and is sandwiched between two other layers to form a so-called pn-junction with them. In this layer, positive (p) and negative (n) charge carriers are created when incident sunlight is absorbed. The most efficient thin-film solar cells to date are based on chalcopyrites, where the light-sensitive layer contains indium and gallium, among other materials. These make the solar cells expensive, and are furthermore classified as critical in terms of long-term availability. Researchers worldwide are therefore looking for better alternatives.

Promising and widely available materials

Especially promising are copper compounds containing the widely available, non-toxic and low-cost elements zinc and tin. "Thin-film solar cells with these substances, however, only reach about 12.6 percent efficiency, maximum," reports Galina Gurieva from the group of Susan Schorr. This is far lower than the efficiency of chalcopyrite cells, which convert more than 20 percent of solar energy into electrical energy. The Berlin material researchers now want to improve the efficiency of zinc and tin-based cells by optimising the chemical composition of the compounds. The trouble is that "so far, next to nothing is known about the fundamental structural properties of these materials, such as atomic defects in the crystalline structure," Gurieva observes. This is because compounds containing both copper and zinc cannot be studied by x-ray diffraction, the traditional method of choice for crystal structure analysis, since the two metals scatter x-ray light very similarly and are therefore almost indistinguishable when analysing the data.



Picture of a kesterite structure containing selenium (yellow), copper (blue), zinc (orange) and tin (red).

Looking for defects with neutrons

The HZB scientists therefore employed neutrons instead of x-ray light to gain new insights. In their scattering experiments with these electrically neutral particles, they used a mixed compound with the complex chemical formula $Cu_{2.04}Zn_{0.91}Sn_{1.05}S_{2.08}Se_{1.92}$. It was previously known that compounds containing only either zinc (Zn) or tin (Sn) in addition to copper, sulphur and selenium crystallise into a so-called kesterite form – a structure that has proven favourable for use in solar absorber layers. The special semiconductor properties of these compounds are determined above all by defects such as disorder in the atomic structure. Yet it was unknown whether a crystal containing copper, zinc and tin would exhibit such disorder.

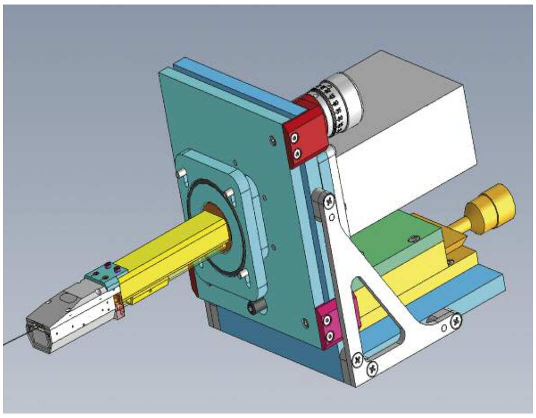
"Using neutron scattering, we managed to solve the puzzle," Galina Gurieva is pleased to announce. The results of their elaborate measurements show that "even this material possesses a kesterite structure" – even if a "certain degree of disorder exists" within them, as the scientist describes it. Together with her research colleagues, she managed to identify the crystalline defects responsible for this. "This is important for understanding what exact composition the material must have to make a suitable absorber layer for high-efficiency thin-film solar cells," Gurieva stresses. Her hope is that "it will be possible to tailor optimised crystalline materials in the laboratory in future. They will give a fresh boost to the development of solar cell technologies." *rb*

Phys. Status Solidi C 12, No. 6, 588– 591, 2015 (DOI: 10.1002/pssc.201400307): Structural characterisation of $Cu_{2.04}Zn_{0.91}Sn_{1.05}S_{2.08}Se_{1.92}$; G. Gurieva, M. Dimitrievska, S. Zander, A. Pérez-Rodríguez, V. Izquierdo-Roca and S. Schorr

"MULTI-SPECTRA GLASSES" FOR SCANNING ELECTRON MICROSCOPY

A new kind of reflection zone plate produced by HZB enables lighter elements in material samples to be precisely detected using scanning electron microscopy (SEM). It provides high resolution in the range of 50 to 1120 electronvolts.

The scanning electron microscope is not only used for precisely surveying the surface topology of samples, but also for determining their chemical compositions. This is done by exciting the atoms to fluoresce under irradiation by an electron beam while scanning the sample.



The new WDS instrument is connected to a scanning electron microscope (Zeiss EVO 40).

This secondary emission provides information about the location and type of element, insofar as the analysis is sufficiently precise. However, the lighter elements of the periodic table such as lithium, beryllium, boron, carbon and nitrogen emit secondary fluorescence in an energy range that cannot be sufficiently well resolved by energy dispersive spectrometers (EDS). But these elements play an important part in energy as well as functional materials.

Diffraction instead of refraction

A solution to this problem has now been developed at HZB. Prof. Alexei Erko, head of HZB's Institute for Nanometre Optics and Technology, has previously designed and patented innovative optics using what is known as reflection zone plates. They are employed in synchrotron sources such as BESSY II for analysing soft X-ray radiation. These optics, consisting of several thousand concentric or elliptical structures, do not refract the radiation the way a glass lens does, but instead diffract them so that interference occurs. "Our colleagues from the company IfG Institute for Scientific Instruments had asked me if reflection zone plate optics could also be used in an electron microscope to increase the resolution in the low-energy region. Based on this idea, a research project at the non-profit Institut für angewandte Photonik e.V. and at the company IfG GmbH was started. A subsequent product development project was then executed resulting in a functional prototype of a specialised wavelength dispersive spectrometer (WDS). Using this instrument you can very precisely detect the light elements such as lithium, boron, beryllium, carbon and oxygen with an electron microscope", explains Erko.

A tool for various questions

The spectrometer consists of an array of 17 reflection zone plates covering the energy range of 50 to 1120 electronvolts (eV). To achieve even higher resolution, the scientists produced optics using 200 reflection zone plates to provide nearly continuous spectral measurements in the energy range of 100 to 1000 eV. "High resolution in this energy range is important for detecting lighter elements of the periodic table. That is particularly important for research on energy-related materials such as solar cells, batteries, and solar fuels, as well as catalysts. But it could also be useful in research on magnetic materials and in life sciences. We are very excited about what this new tool can be used for", says Alexei Erko.

arö

Opt Express, Vol. 22, 2014, 16897-902 (DOI: 10.1364/OE.22.016897): New parallel wavelength-dispersive spectrometer based on scanning electron microscope; A. Erko, A. Firsov, R. Gubzhokov, A. Bjeomikhov, A. Günther, N. Langhoff, M. Bretschneider, Y. Höhn and R. Wedell

UNIVERSALITY OF CHARGE ORDER IN CUPRATE SUPERCONDUCTORS

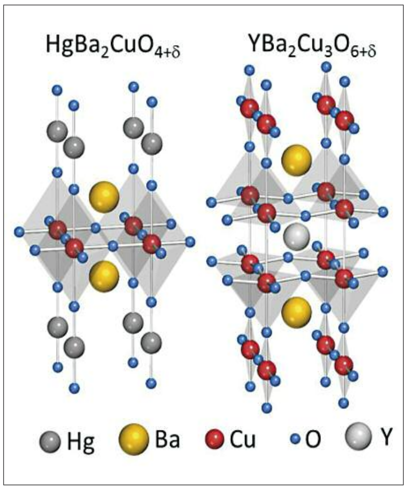
An international research team has identified charge order in an especially **pure high-temperature superconductor** and observed its behaviour in magnetic fields. This brings us a step closer to a better understanding of zero-resistance current flow.

The phenomenon of superconductivity has kept scientists intrigued for decades, and is quite well understood – at least for the classic superconductors, which behave like metals when in non-superconducting state. Superconductivity emerges when electrons pair into so-called Cooper pairs which no longer collide with the crystal lattice and therefore move without resistance. The snag is that it takes temperatures of close to absolute zero, minus 273 degrees Celsius, for this to happen. The same pairing of charge carriers also gives rise to superconductivity in materials called cuprates, but these special ceramics already behave this way at much higher temperatures of minus 140 degrees Celsius, earning them the name of high-temperature superconductors (high-Tc superconductors). Cuprates have one common feature: copper and oxygen atoms are arranged in planes, forming quasi two-dimensional objects. Introducing charge carriers into the copper oxygen planes does not result in a simple metallic behaviour. Rather, a complexity of unusual phases around superconductivity is observed, and how the superconducting state develops from these exotic states of matter has escaped explanation up to now.

Charge carriers form a pattern of stripes

One of the phenomena observed in high-Tc cuprates is the so-called charge order. Here, the charge carriers that are introduced into the ceramics to make them conducting in the first place tend to form a regular pattern of stripes in the copper oxygen planes. Being placed in a regular arrangement renders the charge carrier less mobile and impedes the formation of the superconducting state: charge order is antagonistic to superconductivity. This is of course of the highest importance for exploring the limits of superconductivity and understanding the phenomenon itself. Charge order was observed in one of the cuprate classes already in 1995. It took, however, quite some time to reveal that many other classes of cuprates exhibit the same behaviour. Initiated by researchers from Minnesota, an international team of scientists has now identified charge order in $HgBa_2CuO_4$, emphasizing this universal behaviour.

A further important result of the researchers is the finding that the charge order is closely related to another property of the material. When a very high magnetic field is applied, superconductivity is destroyed, and the electrical resistance goes up and down with changing magnetic field, which is known as quantum oscillations. Finding a universal connection between the period of these quantum oscillations and the spatial period of the charge order is one of the achievements of the scientists. Linking such seemingly distinct observations for a such a complex material is of the utmost importance, as it helps to tell which effect is important and which is only spurious.



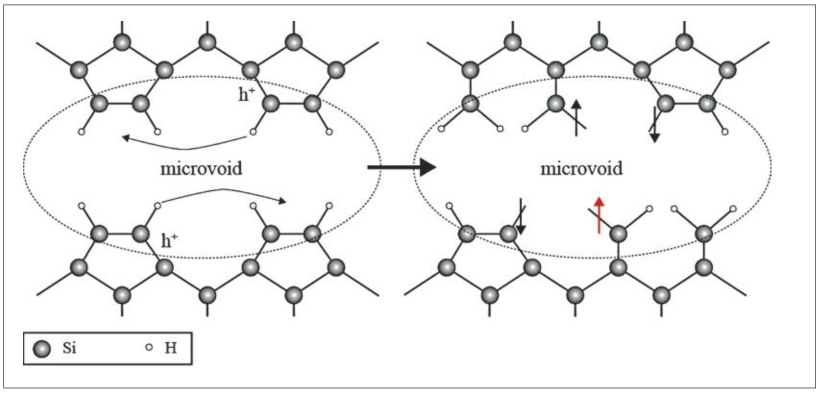
Crystal structures of $HgBa_2CuO_{4+}$ and $YBa_2Cu_3O_6$.

An important part of this research was carried out with the XUV diffractometer at the HZB, employing the particularly sensitive method of resonant soft X-ray diffraction. "After decades of research, the unusual states of matter in the cuprates and their relation to the phenomenon of high-Tc superconductivity are still puzzling the scientists", says Dr. Eugen Weschke from the Department Quantum Phenomena in Novel Materials at HZB." The observation of charge order in this clean model system adds an important piece to the systematics of the cuprates, and we are happy to have contributed to these studies by a number of experiments here at HZB." *Eugen Weschke/arö*

Nature Communications 5, 5875 (DOI: 10.1038/ncomms6875)
Charge order and its connection with Fermi-liquid charge transport in a pristine high-Tc cuprate; W. Tabis et al.

MAGNETIC FINGERPRINTS BRING DEFECTS IN AMORPHOUS SILICON TO LIGHT

Researchers at HZB were able to demonstrate that **tiny voids within the silicon network** are partly responsible for reducing solar cell efficiency by some 10 to 15 percent as soon as you start using them.



In the initial state (left), the voids' internal surfaces are saturated with hydrogen atoms so that no defects are observed. Light-induced charge carriers (h+) destabilize atomic bonds. The breaking of atomic bonds causes defects (indicated by the vertical arrows on the right-hand side), which translates to reduced solar cell efficiency.

Amorphous silicon thin-film solar cells are considered a promising alternative to solar cells based on highly purified silicon wafers, which have been dominating photovoltaic power generation. A major advantage of amorphous silicon thin-film photovoltaics, where a glass substrate is coated with a light-active material less than a thousandth of a millimetre thick, is that the cell fabrication is considerably simpler and much less costly than in the case of conventional crystalline silicon solar cells. On the other hand, a potential disadvantage is the low conversion efficiency from solar energy to electricity. Because of the disordered nature of amorphous silicon, solar cells are subject to the Staebler-Wronski effect, named for the two scientists who first discovered it. It reduces the solar cell efficiency by up to 15 percent within the first 1000 hours.

This undesired effect is triggered by the internal annihilation – known in physics as recombination - of charge that has not been extracted from the solar cell. The released recombination energy induces defects in the amorphous network - which is why this effect is not observed in crystalline wafer solar cells. "However, where defects are produced in the material and whether voids of nanoscale size play a role in all this has not been understood – until now, that is," says HZB's own Matthias Fehr of the Institute for Silicon Photovoltaics. Together with his HZB colleagues, Fehr and scientists from Jülich Research Center and the Free University of Berlin have now made major strides towards unravelling this mystery.

Characteristic magnetic fingerprints revealed

Since the defects that form exhibit paramagnetic properties, they have a characteristic magnetic fingerprint which depends on their microscopic environment. The Berlin researchers were able to identify this fingerprint using electron-paramagnetic resonance (EPR) spectroscopy and electron-spin echo (ESE) experiments. With the help of these highly sensitive techniques, they determined that defects in amorphous silicon actually come in two types: those that are uniformly distributed and those that are concentrated in clusters on internal surfaces of small voids - known in scientific circles as microvoids - which form within the material during the solar cell manufacturing process. "Our guess is that clusters of defects are generated on the internal walls of microvoids which have a diameter of a mere one to two nanometres," explains HZB physicist Fehr. "Our findings seem to suggest that microvoids most likely contribute to light-induced degradation of amorphous silicon thin-film solar cells. For us, it's been a leap forward towards a better understanding of the microscopic mechanism of light-induced degradation," says Fehr. A new series of experiments has been designed to allow the researchers to glean further insights into the atomic and electronic processes of the Staebler-Wronski effect. *rb*

Phys. Rev. Lett. 112, 066403 (DOI: 10.1103/PhysRevLett.112.066403): Metastable defect formation at microvoids identified as a source of light-induced degradation in a-Si:H; M. Fehr et. al.

ORGANIC LAYER ADDS LIGHT PARTICLES

Every solar cell only uses a small part of the solar spectrum. One approach towards circumventing those losses and using more "colours" of the sunlight is photonic upconversion: The solar cell's backside is coated with a material which can add up low-energy photons to yield higher-energy photons which are radiated back towards the solar cell, thus expanding its current harvest. Since 2011, HZB scientists around Prof. Dr. Klaus Lips are collaborating with The University of New South Wales (Sydney, Australia) in investigating novel upconversion materials (see also Highlight Report 2012, p. 37).

The novel class of organic upconversion materials is based on so-called triplet-triplet annihilation (TTA). Together with the Australian partners around Prof. Timothy Schmidt, Dr. Tim Schulze has also investigated the longevity of the TTA molecules under illumination – an extremely critical property for organic materials. The results are promising: even the present not optimized system would last for some years behind a solar cell. At the same time the group reports new record values for the photocurrent enhancement of upconversion-assisted solar cells. "TTA upconversion is a generic optical technology with potential applications beyond thin-film solar cells. They could also assist photo-electrochemical water splitting or organic LEDs," Lips explains. The collaboration with Sydney will continue. *arö*

Energy Environ. Sci., 2015, 8, 103-125 (DOI: 10.1039/C4EE02481H): Photochemical upconversion: present status and prospects for its application to solar energy conversion; T. F. Schulze and T. W. Schmidt

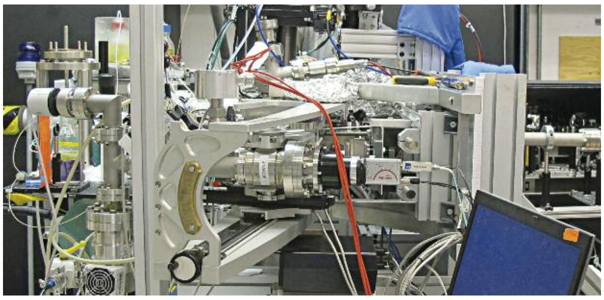
NEW LIGHT ON THE "SPLIT PEAK"

Scientists at the HZB have arrived at a better understanding of how to interpret the electronic and molecular structural dynamics of complex fluids and materials in **X-ray spectra (RIXS)**. In doing so, they have also explained the little-understood and quite controversial phenomenon called the "split peak".

In the last few years, scientists probing the electronic structure of materials can make use of a relatively new technique called resonant inelastic soft X-ray scattering (RIXS). In RIXS, low-energy X-rays from synchrotron or X-ray free-electron laser light sources scatter off molecules within the studied material. If those molecules include light elements, such as the -OH group in alcohols, the complex spectra RIXS produces are difficult to interpret. Controversy has surrounded the split peak structures. The prevailing interpretation has been that spectra revealed some twin aspect of the materials - a split signal related to two separate structures within the molecules. But now a team of researchers from HZB has performed an investigation of several types of liquid alcohols with RIXS and brought new perspective to this long-lasting debate.

X-rays "push" atoms

The researchers were able to demonstrate that the split peaks are tied to dynamic motions produced in response to the scattering X-rays themselves. "We found that the split peak structure in the RIXS spectra of liquid alcohols originates predominantly from nuclear dynamics during the RIXS process," said Simon Schreck, a researcher with the Institute for Methods and Instrumentation for Synchrotron Radiation Research at the HZB and with the University of Potsdam. This insight now provides a meaningful interpretation of the often complicated RIXS spectra and extends the utility of the technique for analysing molecular and electronic structures and their dynamics in complex material systems. *Jason Bardi/arö*



RIXS spectroscopy is a powerful method to gain insights into molecular and electronic structures in complex samples. HZB scientists now know even a bit better how to interpret the RIXS spectra.

Struct. Dyn. 1, 054901 (DOI: 10.1063/1.4897981): Dynamics of the OH-group and the electronic structure of liquid alcohols; S. Schreck et. al.

WARPING IN TOPOLOGICAL INSULATORS

In the POF programme "Future Information Technologies FIT", HZB physicists led by Dr. Jaime Sánchez-Barriga have studied for the first time whether the direction of travel of **electrons in topological insulators** (TI) influences their behaviour. Their results could lead to improvements in the new material class, which could be used for novel components in future information technologies.

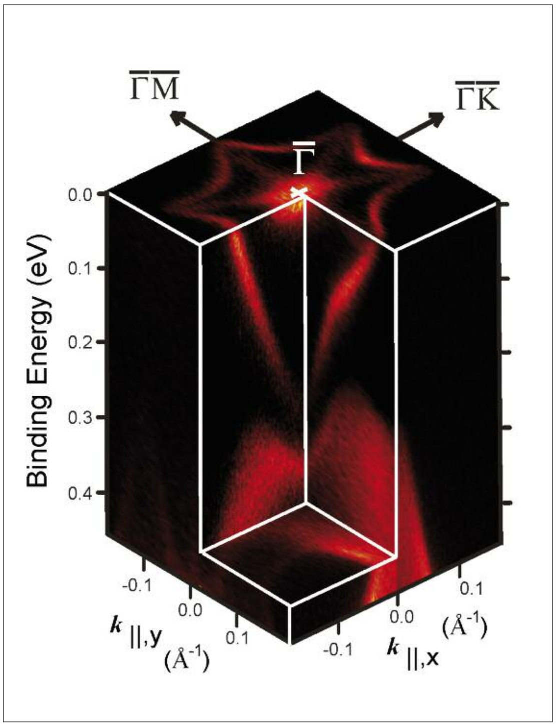
The surfaces of topological insulators conduct electricity in principle without losses, i.e., the electrons manage to avoid hitting obstructions. Nevertheless, experts worldwide are asking themselves why this avoidance does not show up pronouncedly in the experiment. The HZB team with Jaime Sánchez-Barriga were able to show by simulation that the experimental data on the energy distribution of electrons are better explained when the spin of the electrons is considered.
To this end, they investigated the so-called warping of the Fermi surface which describes the energy distribution of the conduction electrons. This is not overly related to warp drive of the science fiction progamme Star Trek since it is not space-time that is bent but the relationship between the energy and momentum of electrons at the surface of topological insulators. However, like in space-time they deal with a light cone, the so-called Dirac cone, because the electrons in topological insulators behave almost like light.

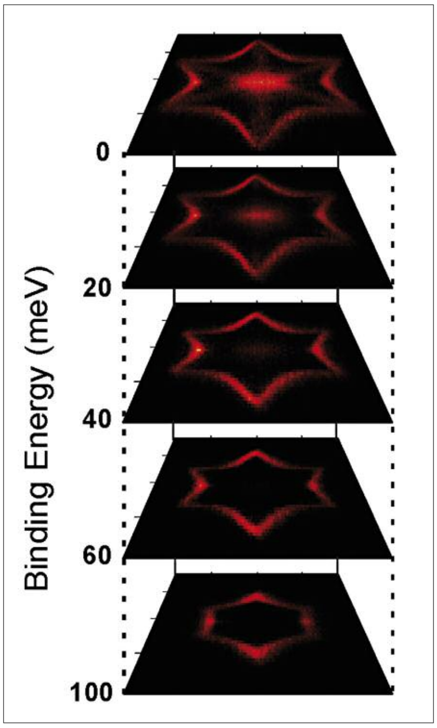
Electron speed depends on the direction

In an ideal Dirac cone, the electrons move with the same speed in all directions, like a soccer ball; still air provided, they will roll equally fast in all cardinal directions. The material bismuth telluride is, however, known for a strong direction dependence of the electron velocity. Sánchez-Barriga and coworkers now discovered that this dependence is a bit different from the expectation. This means that the Dirac cone is not bent inwards but outwards, and although electrons at the surface of topological insulators should not suffer any collisions with obstructions, these collisions do appear in experiments: the Dirac cone appears washed out and with thicker walls.
Sánchez-Barriga and coworkers discovered that this broadening in the warped Dirac cone of bismuth telluride also depends on the direction. This dependence has to be explained first before the limits of lossless transport can be understood. This however, required much scrutiny. At first,

THE DFG PRIORITY PROGRAMME "TOPOLOGICAL INSULATORS"

The discoveries of the quantum spin Hall effect and of topological insulators (TI) have established a new material class in two and three dimensions. Topological insulators are materials which are bulk insulators but exhibit conducting topologically protected surface states. Currently, for only a few materials has the electronic band structure of a TI been demonstrated, and even less systems show experimentally accessible surface states, despite the fact that the number of predicted TI materials is constantly increasing.
The priority programme of the Deutsche Forschungsgemeinschaft (DFG), headed by Prof. Oliver Rader, has been in place since 2013 to drive significant progress in three core areas: advancing existing TI materials, researching fundamental properties and component structures, and discovering new materials and concepts. The focus programme unites German research groups in the field of two- and three-dimensional TIs, in particular bringing experimental and theoretical groups together. The aim is to improve the currently available materials so as to allow room-temperature applications taking advantage of the one- or two-dimensional surface state. This requires continuing study of the growth and of the geometric and electronic structure of the topological insulators. The fundamental properties of TIs yield many extraordinary electronic properties, one example being forbidden backscatter. Studying these properties is important because device structures and measuring techniques, in particular for spin-dependent transport phenomena, can then be derived for exploitation in future electronic components. New materials such as oxides can help overcome the limitations of currently known TI materials and even bring new, useful properties with them. *cn*





Both figures display experimental data on the "Dirac cone". The outward warping is pronounced as well as the broadening of the boundaries of the cone which is caused by collisions of the electrons with obstructions in the real, non-ideal, topological insulator bismuth telluride.

it must be excluded that the different velocities, i.e., the very warping, cause the different scattering behaviour, corresponding to the expectation that a faster ball is more likely to miss its path.

The impact of spins

The simplest explanation is the so-called nesting. The nesting of a warped Dirac cone is high if its outline consists of many sections that are parallel to each other on opposite sides. This is maximally the case for a square and a hexagon, hardly for a circle and absent for a triangle.
Sánchez-Barriga and coworkers were unable to reconcile their results with nesting. Therefore, they searched for factors neglected so far and considered the spin, the angular momentum, of the electrons. Using the example of the kicked ball: "For bismuth telluride, the ball does not only roll faster when I kick it northwards as compared to eastwards. Only eastwards does it roll normally, northwards one cannot call it rolling since its spin axis points a bit skywards like a cut ball in football," Jaime Sánchez-Barriga explains. The scientists performed simulations and only considering this spin, they were able to reproduce their experimental results.

New possibilities with BESSY-VSR

The losses due to collisions can also be viewed as lifetime of the electrons which apparently depends on the direction. These dynamic effects occur on an extremely short timescale and shall be investigated with time resolution next. This research will profit largely from the possibilities of a future BESSY-VSR light source. The published experiments have been conducted in the framework of the Helmholtz-Russia Joint Research Group of Andrei Varykhalov and are part of the DFG Priority Programme "Topological Insulators" which is coordinated by Oliver Rader.

arö

Phys. Rev. B 90, 195413 (DOI: 10.1103/PhysRevB.90.195413): Anisotropic effect of warping on the lifetime broadening of topological surface states in angle-resolved photoemission from Bi_2Te_3; J. Sánchez-Barriga, M. R. Scholz, E. Golias, E. Rienks, D. Marchenko, A. Varykhalov, L. V. Yashina and O. Rader

IN BRIEF

- HZB physicists have studied how electron behaviour in a topological insulator (TI) changes depending on the electrons' direction of motion.
- They identified directions in which the electrons are much more susceptible to scatter loss, and electric conductivity is therefore hindered.
- To explain their results, they factored in the spin of the electrons for the first time, and in doing so challenged a dominating paradigm.
- The results could provide a boost in the research of topological insulators, especially when significantly shorter light pulses become available at BESSY-VSR for studying the electron dynamics.

PRODUCING HYDROGEN IN TANDEM

In the scope of programme-oriented research at the HZB, scientists led by Prof. Roel van de Krol, Head of the Institute for Solar Fuels, together with researchers from Delft University of Technology, have used novel bismuth vanadium oxide layers in various components to **obtain hydrogen**.

Hydrogen is most commonly produced by splitting water using electric current. An especially simple method involves photoelectrochemical cells, where electricity generated from sunlight serves directly to split water molecules apart. Such a system employs tandem cells – a combination of several different solar cells each optimised to convert a different part of the solar spectrum into electrical energy. Suitable materials for the electrodes, where the actual electrochemical splitting of water takes place, include metal oxides such as titanium dioxide (TiO_2), iron oxide (Fe_2O_3) and bismuth vanadium oxide ($BiVO_4$).
Prof. Roel van de Krol and his team combined thin bismuth-containing layers with a micromorphous silicon solar cell (a-Si/µc-Si) that unified a blue and a red light absorber. With this tandem cell, the researchers managed to set a new efficiency record for solar hydrogen production: They converted 5.2 percent of the energy from sunlight into hydrogen. They achieved this by doping the $BiVO_4$ with tungsten atoms at a certain density distribution and applied the electrodes onto a substrate with a structured surface that captured the sunlight for the electricity generation.
In another project, the HZB researchers collaborated with a team of the Swiss École polytechnique fédérale in Lausanne (EPFL). Again, the centrepiece was a photoelectrode made of $BiVO_4$. The researchers combined this with a copper oxide counter electrode (Cu_2O) into a tandem system consisting exclusively of oxide materials. Theoretically, this should allow them to obtain solar hydrogen at an efficiency of up to eight percent. While their experiments have yielded an efficiency of only one percent so far, the team has confirmed that the combination of $BiVO_4$ and Cu_2O is in principle suitable for photoelectrochemical splitting of water. The trouble was, the catalyst material the researchers had integrated into the cell to support the chemical reactions dissolved too quickly. “With an alternative catalyst, however, we will be able to overcome this instability of the system,” Roel van de Krol is convinced. *rb*

Hydrogen is considered an excellent storage and transport medium for energy derived from sunlight. Car manufacturers such as BMW are developing vehicles with engines using hydrogen.

ChemSusChem 2014, 7, 2832 – 2838 (DOI: 10.1002/cssc.201402456): Efficient Water-Splitting Device Based on a Bismuth Vanadate Photoanode and Thin-Film Silicon Solar Cells; L. Han et. al. and J. Phys. Chem. C 2014, 118, 16959–16966 (DOI: 10.1021/jp500441h): A Bismuth Vanadate–Cuprous Oxide Tandem Cell for Overall Solar Water Splitting; P. Bornoz et. al.

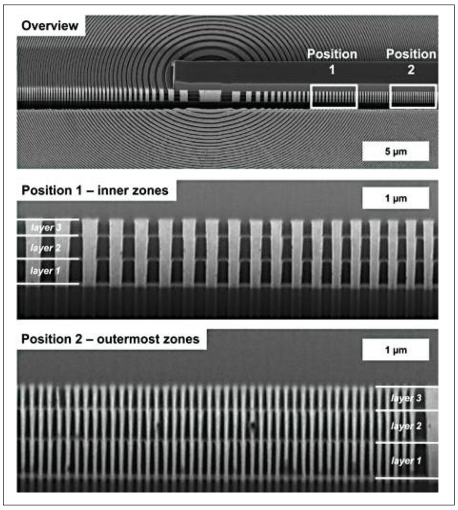
TITANIUM DIOXIDE SLOWS DOWN UNWANTED RECOMBINATION

The efficiency of perovskite-based solar cells has increased from 3 to 16 percent over a period of a few years. Yet, the processes occurring in the cells are still barely understood. Researchers at the EPFL and at the HZB Institute for Solar Fuels have managed to explain two central processes using time-resolved spectroscopy: The separation of charge by sunlight always takes place in less than one picosecond. Yet, an unwanted process called recombination reduces the efficiency, and greatly depends on the materials used. It turns out recombination happens much slower in titanium dioxide than in aluminium trioxide. This insight will help in the targeted design of higher efficiency solar cells.

SHARPER IMAGING USING X-RAYS

Physicists at HZB have developed a process to generate improved lenses for X-ray microscopy that provide both **better resolution and higher throughput**.

The wavelength of light limits resolution in microscopy. Visible light can resolve structures on the order of a quarter-micron, while the considerably shorter wavelength of X-rays can in principle resolve features down to a few nanometres. In addition, X-rays can also penetrate more deeply into specimens, so that internal structures of three-dimensional specimens can be investigated. However, though light in the visible region can be focused using refractive lenses made of glass, this approach does not work with soft X-rays. In order to utilise X-rays for imaging, it is necessary to use Fresnel zone plates, which are made out of concentric rings composed of metals such as nickel or gold. These metal rings diffract X-rays so that contributions from the different zones are constructively superposed at the focal point. The result is that Fresnel zone plates act as objective lenses to focus X-rays and can be employed in X-ray microscopes. The achievable spatial resolution depends on the smallest ring width that can be manufactured, which up to now has been about ten nanometres.
An improvement of spatial resolution to below ten nanometres poses both technological and fundamental physical problems. On the one hand, it is technologically extremely challenging to fabricate periodic zone structures having a ring width of less than ten nanometres and a height of a few hundred nanometres. On the other hand, theoretical calculations indicate that with decreasing ring width, these types of optics would be increasingly inefficient and would simply collect too little light. This dilemma can be resolved with the help of volume diffraction. However, the approach requires zone features that simultaneously have an increasing tilt angle and a declining zone height versus radius, i.e. three-dimensional structured X-ray optics. “Theoretically, though, almost 100 per cent of the incident light could be utilised for the image,” explains Dr. Stephan Werner from the Microscopy Research Group at the HZB Institute for Soft Matter and Functional Materials.



These scanning electron micrographs show how accurately the three Fresnel zone plates were positioned above one another. 3D X-ray optics of this kind allow the resolutions and optical intensities to be considerably improved.

Precise stacks of Fresnel zone plates

In a first step towards three-dimensional X-ray optics, the experts at HZB have manufactured three layers of Fresnel zone plates nearly perfectly above one another. “We have developed a process that enables on-chip stacking of Fresnel zone plates with a precision of less than two nanometres,” says Dr. Gerd Schneider, who heads the Microscopy Research Group. The initial measurements demonstrate that this structure captures considerably more light for imaging than conventional Fresnel zone plates. “If we are successful in positioning five zone plate layers above one another, which is our next goal, we will be able to utilise a many-times-higher fraction of the incident X-ray light for imaging than has been available up to now,” says Werner.
X-ray microscopy is an important technique for a wide range of research topics, for example in the life sciences to investigate cell organelles, viruses, and nanoparticles within cells, as well as for materials science and energy research to study novel electrochemical energy storage approaches in situ. Users at BESSY II could soon be profiting from this advance as well. *arö*

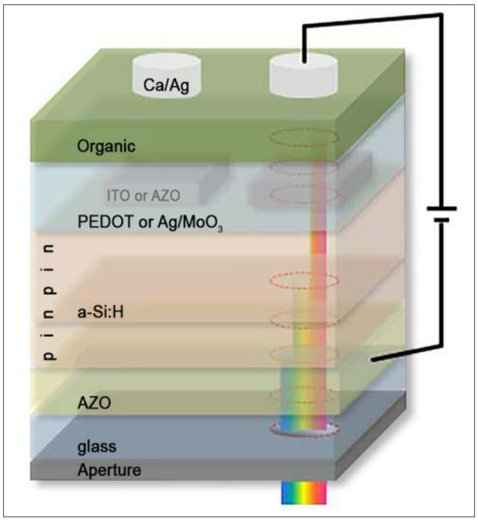
Nano Research 2014, 7(4): 528–535 (DOI: 10.1007/s12274-014-0419-x): Three-dimensional structured on-chip stacked zone plates for nanoscale X-ray imaging with high efficiency; S. Werner et. al.

MAXIMUM EFFICIENCY, MINIMUM MATERIALS AND COMPLEXITY

Two research groups at PVcomB have improved the **efficiency of thin-film solar cells**. A hybrid thin-film solar cell newly developed at the PVcomB achieved a record efficiency of more than eleven percent. The researchers have also succeeded in improving the absorber for solar cells made of chalcopyrites.

Thin-film silicon solar cells use 10 to 100 times less silicon than classic crystalline wafers. The HZB Competence Centre Thin-Film and Nanotechnology for Photovoltaics Berlin (PVcomB), headed by Prof. Rutger Schlatmann, is dedicated to developing these technologies. Together with a team from the University of Potsdam, led by Prof. Dieter Neher, the PVcomB has come up with a hybrid stacked cell that combines inorganic and organic materials. In this configuration, the solar cell can not only use photons in the blue and green range of the light spectrum, but can also convert the red and infrared light of the sun's energy into electrical current.

This hybrid organic/inorganic triple cell achieves an efficiency of over eleven percent – a significant increase compared to a pure a-Si:H solar cell, the efficiency of which is typically between seven and eight percent. "The cell can be fabricated easily with established thin-film technology common in the industry, and is also suited to production in large sheets," says Schlatmann. Neher adds: "The high absorption coefficients of a-Si:H layers and the properties of the organic layer make possible an active stack no thicker than one micron – that is maximum efficiency with minimum materials." Two junior scientists from the two institutes were significantly involved in the development: Steffen Roland of the University of Potsdam and Sebastian Neubert of the PVcomB.



The a-Si:H is deposited on an AZO film that acts as a transparent front contact. An ITO layer serves as rear contact. The organic subcell possesses a front contact made of a conductive polymer material (PEDOT) and a metallic rear contact.

Optimisation factors for flexible solar cells

A promising alternative to the widely used crystalline silicon are semiconductor materials made from chalcopyrite compounds such as copper-indium-gallium-diselenide (CIGSe). At the PVcomB, scientists have now studied what factors have a positive influence on the efficiency when producing CIGSe absorbers on a plastic film. They applied the semiconductor as a film two to three micrometres thick onto a flexible polyimide film. This especially light substrate remains stable at relatively high temperatures of around 450° Celsius. "Other flexible substrates such as metals are expensive, somewhat heavier, not quite as flexible, and run the risk of contaminating the semiconductor material at high temperatures," explains Christian Kaufmann, who coordinated the joint project. "The aim of the current research at PVcomB is to optimise those aspects that determine the quality of the CIGSe absorber for lower temperatures," project team member Dieter Greiner explains.

Given a better understanding of the CIGSe growth process, the researchers have managed to lower the selenium consumption in the manufacturing process, shorten the processing time and improve the absorber layer. "Also, reducing the zinc oxide layer thickness in the transparent front contact has helped increase the efficiency to 17.9 percent," says Greiner. The thin-film solar cells made of copper-indium-gallium-diselenide compounds are therefore not only potentially cheaper than those made of polycrystalline silicon; they may even one day surpass their silicon siblings in efficiency. *tm/arö*

Adv. Mater., 27: 1262–1267. (DOI: 10.1002/adma.201404698): Hybrid Organic/Inorganic Thin-Film Multijunction Solar Cells Exceeding 11 percent Power Conversion Efficiency: S. Roland, et. al. and Presentation at the 42. IEEE Photovoltaics Specialists Conference: Optimizing the Growth Path for Cu(In,Ga)Se_2 Thin Films Co-Evaporated at low Temperatures on Flexible Polyimide Film; D. Greiner

X-RAY VIEW INTO THE ELECTROCHEMICAL CELL

Dr. Kathrin Aziz-Lange, scientist at the Institute for Solar Fuels and her team have developed a **novel measuring cell** at the HZB. Inside this cell, electrochemical and catalytic processes can be studied using X-ray spectroscopy in soft X-ray light.

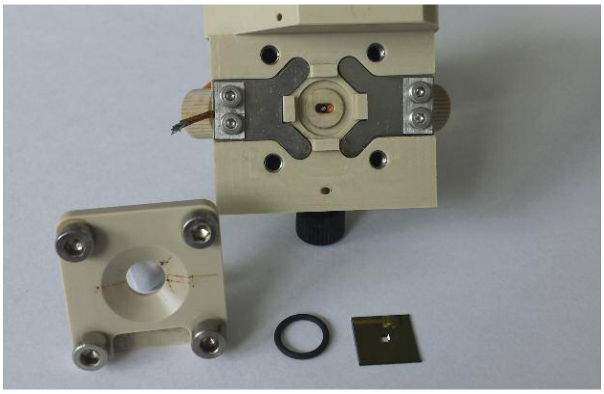
Catalysts that drive electrochemical reactions are a crucial factor in the efficiency of batteries, fuel cells and solar cells. In order to optimise their function, researchers need to know the electronic structure of the materials involved in as much detail as possible. Why and under what conditions are chemical bonds made or broken again? An ideal tool for answering such questions is soft X-ray light – electromagnetic radiation of about 100 to 200 electron volts. It can be used to look deep into the inner life of metal compounds that serve as catalysts, such as ferrous or cobalt-based materials.

"Using soft X-ray light, we can observe the d-orbits of the metals, which are decisive for their chemical bonding and thus for the catalytic action," says Dr. Kathrin Aziz-Lange. The trouble is, because oxygen and nitrogen in the air absorb X-ray radiation, the measurements must be made in a vacuum. Yet, the electrochemical processes of interest take place at the interface between a solid and an electrolytic fluid while a voltage is applied – "for example when dealing with materials that serve to split water," Aziz-Lange explains. "Combining this with radiation in a vacuum is a challenge."

To overcome this challenge, the researchers separated the sample from the surrounding vacuum by a membrane merely 100 nanometres thick. The X-ray light can cross the membrane with ease – and through a 20 nanometre-thick layer of gold applied behind it. This serves as the electrode. An electrical voltage can be applied between it and a counter electrode on the back wall of the measuring cell. The materials to be studied can then be deposited onto the gold from the adjacent electrolyte fluid.

Two methods deliver a wealth of information

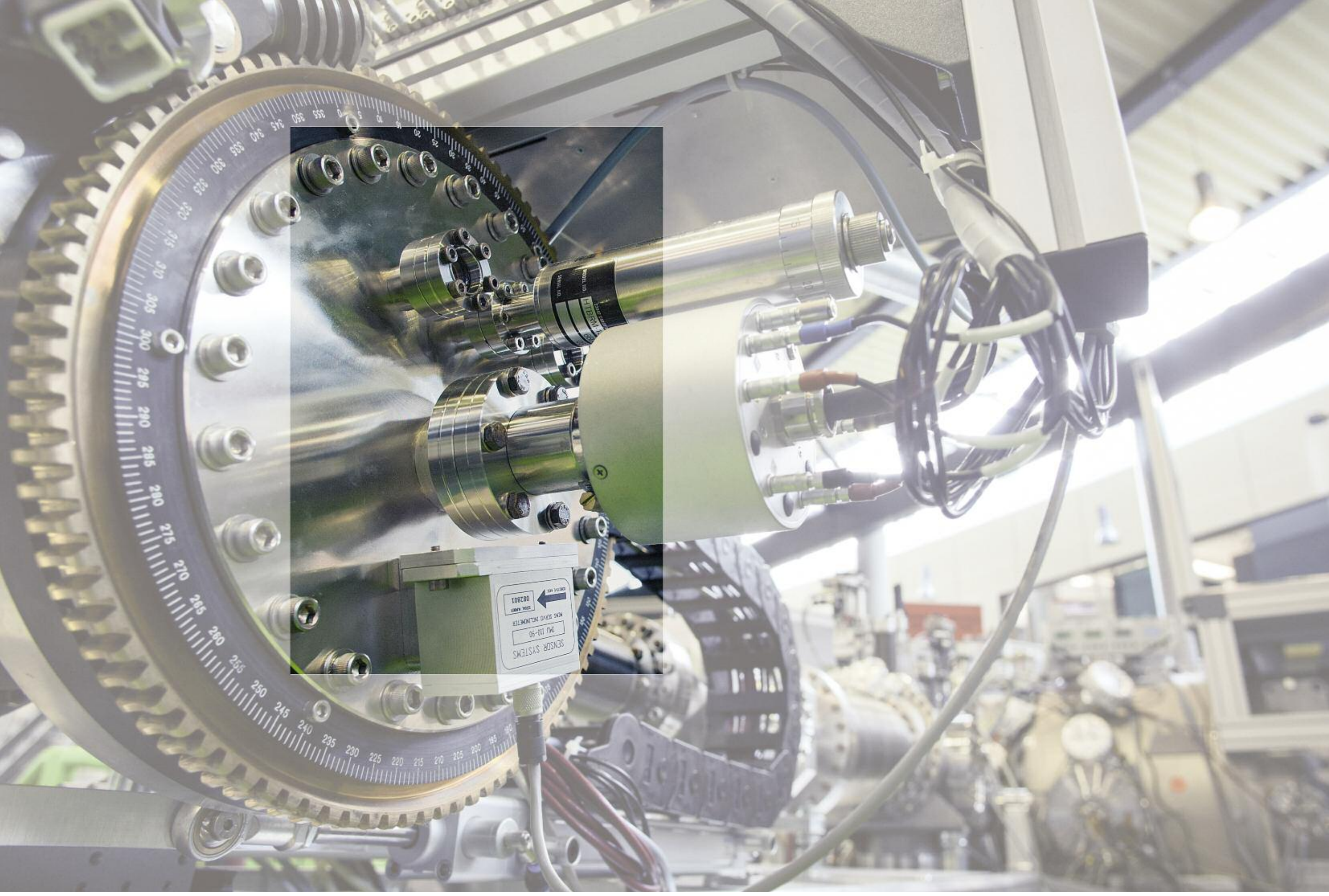
The flow cell can be placed in the LiXEdrom spectrometer at the HZB's storage ring BESSY II, which delivers X-ray light for experiments. Detectors can detect the intensity of fluorescence as a function of both the energy of the exciting photons and the emitted photon energy. "One can now run absorption and emission spectroscopy on electrochemical systems with it," Aziz-Lange announces. Both methods deliver a wealth of information on the electronic properties of the material and chemical reactions taking place in the sample. "Inelastic X-ray scattering even allows us to obtain information on ultrafast processes on the femtosecond timescale," the scientist says.



In the new measuring cell of the LiXEdrom, electrochemical reactions at the interfaces between solids and liquids can now be studied in a vacuum with soft X-rays.

The team demonstrated the functionality of the measuring cell on a cobalt chloride solution. The researchers had this solution flow across the gold surface while an electric current was applied, and observed what happened. The results of the experiment reveal that the cobalt deposited onto the gold – much like when producing catalyst layers. "In the first experiments on catalysts for electrolysis, we analysed here how the electronic structure of the materials change as a function of the applied voltage and in what oxidation and spin state the metal existed," Kathrin Aziz-Lange reports. The researcher is convinced of the benefits of her development: "The interest in the apparatus and the application possibilities are immense." It is available for answering the queries of all interested scientists. *rb*

Rev. Sci. Instrum. 85, 103120, 2014 (DOI: 10.1063/1.4899063):Electrochemical flowcell for in-situ investigations by soft X-ray absorption and emission spectroscopy; C. Schwanke, R. Golnak, J. Xiao and K. M. Lange



JOINT VENTURES

58 new cooperatives were concluded by HZB in 2014. By the end of 2014, there was a total of 249 scientific cooperatives under way.

Together with the Freie Universität Berlin (FUB) and the Zuse Institute Berlin, HZB set up the **Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE)**. BerOSE is meanwhile the tenth “joint lab” at HZB (see page 50). Associated with formation of the joint labs is the promotion of young talent, represented in each case by the appointment of a junior professor.

The **Turkish-German University** in Istanbul has received support from the HZB and the University of Potsdam since 2014. Both institutions are active in the concept and set-up of two Bachelor study courses in the special field of materials science and technology as well as in the lab design and instrument installation.

In December 2014, HZB organised the joint **BER II and BESSY II User Meeting**. More than 500 users of both HZB large-scale facilities came to inform themselves about the latest developments in technology and to exchange ideas on scientific issues.

THE PATH TO ARTIFICIAL PHOTOSYNTHESIS

Scientists at HZB in collaboration with the Monash University, Australia, have precisely characterized a **manganese catalyst's electronic states**. The catalyst is capable of converting light to chemical energy.

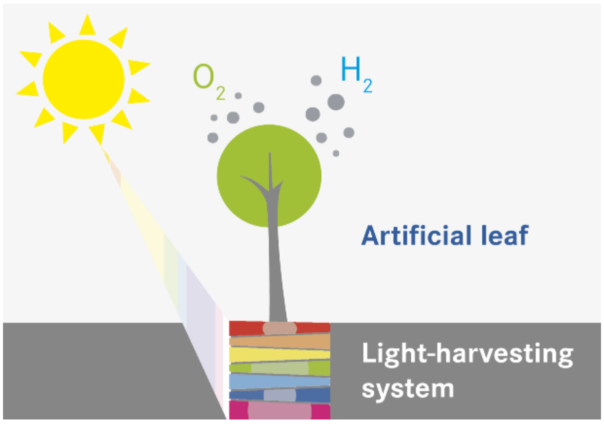
If sunlight could be effortlessly converted to chemical energy, our energy troubles would be a thing of the past. Green plants have evolved a special kind of mechanism to help them do just that: photosynthesis, the process by which plants take sunlight and, with its help, produce high-energy substances such as sugar from water and carbon dioxide. But the molecules located in the so-called "oxygen evolution centre" that facilitate this series of steps inside a plant cell are highly complex and sensitive. A current mission of scientists is simulating them in a laboratory setting and optimizing them for commercial energy production.

At his Institute "Methods for Material Development", Prof. Dr. Emad Aziz is doing research on artificial water splitting catalysts with the goal of getting them to perform at the level of the oxygen evolution centre of photosynthesis.

A while back, the scientists figured out what the chemical nature of these types of energy converters would need to be. Top candidates are manganese complexes embedded in a nafion matrix, a teflon-like polymer. Prof. Leone Spiccia's lab developed and provided the samples. He says: "Under a bias, our manganese complexes produce nanoparticles of manganese oxides within nafion matrix. When exposed to light and biased simultaneously, these oxides promote water oxidation, a key and challenging reaction associated with splitting water into oxygen and hydrogen. The hydrogen can be stored as an energy carrier."

Deep insight into catalytic processes

"The next step was to figure out which of the potential manganese complexes in nafion yields the best manganese oxides," says the scientist in charge of the experiments, Munirah Khan of the Freie Universität Berlin, holder of a DAAD and a Higher Education Commission (Pakistan) scholarship. She studied the formation of manganese oxides and their catalytic effect using X-ray light at BESSY II, the HZB's synchrotron radiation source. In her doctorate research work, Khan used the RIXS method, which allowed her to select and further investigate the manganese species involved in catalytic processes with high precision.



Artificial catalysts imitate natural photosynthesis.

Of the various manganese complexes, one in particular – designated Mn(III) by the scientists – turned out to be the one that most efficiently formed manganese oxides. "We are developing our methods to construct multi-dimensional catalytic pathways for such novel materials in the energy and timescales. Our goal is to provide synthetic chemists with a full picture of the catalytic process under real test conditions in order to enhance their work on the function of these materials," says Emad Aziz, "and figure out if and under what conditions it might be used for technological application in converting light to chemical energy. If we succeed, it could mean we're well on our way towards a continuous, environmentally friendly and cost-effective storage form of solar energy." *hs*

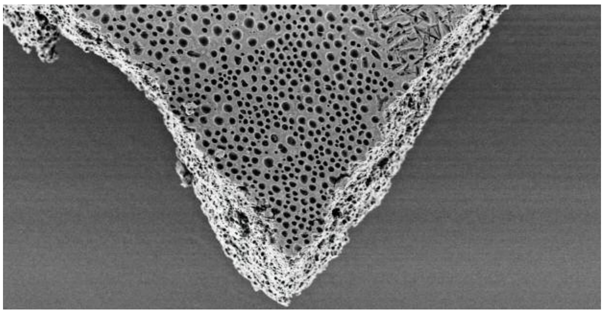
ChemSUSChem, Vol. 8, 5, 872-877 (DOI: 10.1002/cssc.201403219): Enhancing Catalytic Activity by Narrowing Local Energy Gaps–X-Ray Studies of a Manganese Water Oxidation Catalyst; J. Xiao, M. Khan, A. Singh, E. Suljoti, L. Spiccia and E.F. Aziz

J. Mater. Chem. A, 2014,2, 18199-18203 (DOI: 10.1039/C4TA04185B): Electronic structural insights into efficient MnOx catalysts; M. Khan, E. Suljoti, A. Singh, S.A. Bonke, T. Brandenburg, K. Atak, R. Golnak, L. Spiccia and E.F. Aziz

SIMPLE FORMULAE FOR COMPLEX BEHAVIOUR

In a cooperative project with chemists of the MPI of Colloids and Interfaces in Golm, HZB physicist Prof. Joachim Dzubiella analysed the mechanical properties of **biomimetic materials** with the aid of computer simulations.

Sea cucumbers change the stiffness of their skin, Venus flytraps roll up their leaves and even pine cones are capable of closing up their scales at increasing levels of humidity. In the course of evolution, Nature has managed to give rise to complex materials capable of responding to external stimuli by way of mechanical movement. Which is exactly what chemists are now trying to do as well – and with considerable success. Dr. Jiayin Yuan's team at the MPI of Colloids and Interfaces recently managed to synthesize a membrane capable of rolling up extremely rapidly when exposed to fumes. Now, Joachim Dzubiella, a



A talent for motion: thanks to its pores and chemical structure, the biomimetic membrane developed by the scientists from the Max Planck Institute of Colloids and Interfaces curls faster and more vigorously than comparable materials.

theoretical physicist at the HZB, has managed to identify those factors that are responsible for the high speed.
The porous material consists of interconnected polymers. Here, polymers in the top layers are visibly more tightly interconnected than is true of the bottom layers. And when the membrane takes up certain gas molecules such as acetone, it bulges more strongly at the top than it does at the bottom, so that it starts to warp, ultimately coiling up. “Jiayin Yuan and his team have already characterized the phenomena in much depth, and we were able to pick up where they left off,” explains Dzubiella, prompting him to propose that the gas molecules initially cross the membrane by “diffusing” across it. The time it takes them to penetrate the membrane depends both on the size of the pores as well as on the thickness of the membrane. The larger the pores and the thinner the membrane, the faster the gas molecules are able to cross. The chemists had already witnessed this behaviour in the lab.

Thin membranes bend faster

Dzubiella also managed to show why it is that the membrane literally curls up when exposed to the vapour, in other words, why it exhibits a particularly small radius of curvature: “We're talking simple geometry,” he says. “If the membrane is really thin, very small expansions of the top layers are enough to cause strong bending.” Within one-tenth of a second, the membrane bends into a full circle; within a half a second, it is rolled up multiple times. Which is ten times faster than is true of similar materials.
Together with his postdoc, Dr. Jan Heyda, Dzubiella is continuing his work using a computer to simulate the movement and embedding of gas molecules within the membrane’s network. The reason being that, at a microscopic level, the processes are rather complex and especially between the polymeric molecules and the gases, very different types of interactions are able to take place. As such, the polymer network also takes up water molecules from the humidity in the atmosphere. If the membrane now comes into contact with acetone, the acetone molecules migrate into the network, displacing the water molecules. “Oftentimes, it is only by way of simulations that we’re able to show the ways in which this could be happening and which processes and factors are important here. These insights in turn are helping the chemists optimize a given parameter in the lab in order to reach the desired property,” explains Dzubiella.
In terms of potential applications, the sky is the limit. For example, you might coat other types of materials with these kinds of membranes which begin to fold up as soon as they come into contact with certain molecules. Already, the chemists were able to document that the rolling up not only works with acetone but even with French perfume. *arö*

Nature Communications, 5, 4293 (DOI: 10.1038/ncomms5293): An instant multi-responsive porous polymer actuator driven by solvent molecule sorption; Q. Zhao et. al.

AMORPHOUS TURNS CRYSTALLINE

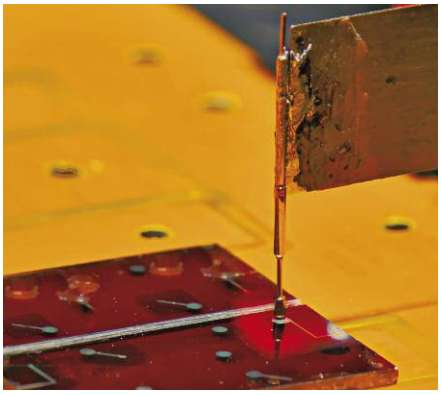
In cooperation with Evonik Industries, HZB scientists have tested the practicality of a liquid silicon compound, showing that it can be used to produce **crystalline thin-film solar cells** in a simple process.

The efficiency and manufacturing costs of photoactive layers are key success factors for the solar technology. A promising method requiring low material and energy input is to manufacture the photoactive layer out of a liquid silicon compound. One starting material that seems to fit the bill is the compound neopentasilane. Specialist chemicals company Evonik developed the compound; HZB experts tested its applicability.

In a first experimental set-up, a group working with Dr. Tobias Sontheimer put a neopentasilane film of only a few microns thickness on glass through a certain process. "Our aim was to convert this amorphous silicon into crystalline silicon using a relatively simple and low-cost method," Dr. Daniel Amkreutz of the project group explains. The HZB scientists used a scalable beam source – one that can be easily scaled up for larger substrates – to heat the substrate locally to 1400 degrees Celsius. "The accelerated electrons heat the silicon so much that the layer melts locally and then hardens again in alignment. That way, electrical losses are minimised and efficiency is increased," Amkreutz describes the process. The result is a preparation that works like a conventional solar cell.

Effective passivation yields higher-efficiency heterojunction solar cells

In a second experimental set-up, they deposited the neopentasilane as a thin, amorphous silicon film onto a monocrystalline silicon wafer. These amorphous/crystalline silicon heterojunction solar cells allow for excellent passivation, a critical factor for the efficiency of a solar cell. "What passivation does is ensure that only a few of the charge carriers generated by the sunlight on the outer surface of the solar cell are lost again to the process of recombination," HZB scientist Mathias Mews explains. While the surface of crystalline silicon has many dangling bonds, where recombination takes place, the amorphous silicon is very hydrogen-rich and therefore has no dangling bonds at its surfaces. In an amorphous/crystalline silicon solar cell, the amorphous layer therefore seals the wafer on the outside. *tm*



Solar cells made of a liquid silicon compound – shown is a specimen from a cooperative between Evonik and the Forschungszentrum Jülich – promise higher efficiency levels at lower costs.

Adv. Mat. Interfaces, 2014, 1, 1300046 (DOI: 10.1002/admi.201300046): Solution-Processed Crystalline Silicon Thin-Film Solar Cells; T. Sontheimer et. al. and Appl. Phys. Lett., 2014, 105, 122113 (DOI: 10.1063/1.4896687): Solution-processed amorphous silicon surface passivation layers; M. Mews et. al.

NANOPARTICLES YIELD EVEN THINNER SOLAR CELLS

Thin-film solar cells made of chalcopyrite (CIGS) consist in part of expensive rare-earth elements such as indium and gallium. If the active layer is made too thin, the efficiency level drops. Nanostructures might be able to capture the light and thus increase the efficiency. This idea is being pursued by Prof. Martina Schmid, who heads the Nano-optiX group of junior scientists at HZB and holds a junior professorship at Freie University Berlin. One option to achieve this is to construct simple nanostructures from metallic particles. In collaboration with colleagues at the California Institute of Technology, Schmid investigated how these types of randomly distributed nanoparticles influence the incidence of light on a cell below. Her work points the way for improved designs of these nanostructures. *arö*

TAILORED DISORDER

Prof. Dr. Silke Christiansen is a scientist at HZB, FU Berlin and Max Planck Institute for the science of light, and coordinates the new DFG priority programme **"Tailored Disorder"**. It's task is to enhance innovative solutions for solar cells, optical elements and surfaces.

The last several years have witnessed considerable progress in the field of nanooptics. Up until now, a maximum degree of regularity was thought to be a prerequisite for perfect functionality – although nature itself yields a host of templates for how tailored disorder can be implemented on the smallest of structural scales. As such, the exact same starting material may produce the vibrant colours of the wings of a butterfly while in beetles of the family Cyphochilus it yields a brilliant white, regularly scattered surface with an underlying three-dimensional nanoarchitecture. Only over the last couple of years have irregular structures been probed systematically for their potential relevance to optical applications. The first set of publications on the topic documents the mind-boggling potential of random nanostructures such as the world's smallest disorder-based spectrometer.

Whether a surface – like the butterfly's wing pictured here – shimmers colourfully or appears evenly white depends on its nanostructure.

To systematically tap the potential inherent in this new class of materials, renowned scientists from a range of disciplines - from biology, physics and chemistry, all the way to computer and even material science - are working side by side as part of the "Tailored Disorder" priority programme's core team. Given this diverse expertise, the theoretical description of complex systems, their numeric simulation, production and modification using nanostructuring (a top-down approach) and chemical synthesis (a bottom-up approach) can be realized to create tailor-made technological applications - from the planning stages through to their large-scale realization.

Improved solar cells, optical elements or special car paints

"If we were able to master these new kinds of materials, it would open up a plethora of possibilities for controlling broadband light since there are far more degrees of freedom in tailored disorder than is true of ordered systems," explains Silke Christiansen. Potential applications range

FATHOMING THE POTENTIAL OF "DISORDER"

The Deutsche Forschungsgemeinschaft (DFG) continues to fund its so-called SPP priority programmes to combine the research efforts in promising fields. One of the 16 priority programmes officially starting in 2015 is the "SPP Tailored Disorder", which will allow the scientists of the institutes involved to develop new materials that exploit the principle of tailored disorder in their structure. The DFG plans to fund the "SPP Tailored Disorder" until 2021 with a total of about 12 million euros.
As a chance for those interested in the topic to network, a kick-off meeting was held in September 2014, with around 65 scientists attending. The programme committee headed by Prof. Christiansen explained the organisation of the priority programme, which is divided into five thematic units: Natural Photonic Systems in Biology, Physics of Disordered Materials, Computational Simulation, Materials Science and Engineering and Interface Chemistry. The participants also presented the concepts for their topics on 40 posters, which were discussed in short lectures. "The meeting served as an occasion for the interested parties to get to know one another and exchange ideas, in order to formulate interesting and promising proposals," Silke Christiansen explains.

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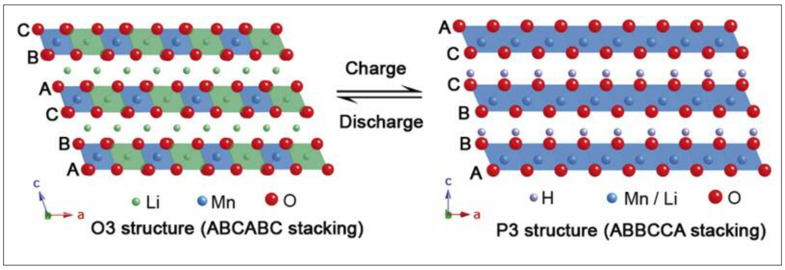
from improved solar cells and novel optical elements all the way to special car paints. And basic science researchers expect they will glean promising new insights they can apply to 3-D Anderson localization or to improving our understanding of random laser properties. Medicine is also bound to benefit from findings that might come out of the "Tailored Disorder" priority programme – for if we understand the scattering properties of organic materials like, say, the human skin, it will be possible to "look through them" as well. *arö*

WHY DO LITHIUM-ION BATTERIES AGE?

A team of researchers at HZB and University of Münster observed atomic rearrangements occurring in the **cathode material of lithium-ion batteries** at the synchrotron sources BESSY II at HZB and DORIS at DESY. They discovered why their capacity diminishes with each charging cycle.



The original structure of the material has an ABCABC arrangement of oxygen layers (left). Due to the Li+H+ exchange during the charging process it degrades to ABBCCA (right).

Rechargeable Li-ion batteries are the power sources of choice for various portable electronic devices such as cellphones, laptops and cameras. "Also, they are gradually finding applications in the automobile industry", Dr. Jatinkumar Rana from HZB says. The young scientist and his colleagues in collaboration with the group of Prof. Martin Winter at University of Münster were interested in elucidating electrochemical processes in high-capacity Li-rich cathode materials. The cathode material is $(x)Li_2MnO_{3*(1-x)}LiMO_2$, and "M" is a transition metal such as Manganese, Chromium or Iron. These materials are the best candidates for the next generation of lithium-ion batteries because they deliver twice the capacity of the commercially available cathode materials and exhibit exceptionally high rate capabilities, so that they can be charged or discharged in short times or at very high currents. "Besides, they contain lesser amounts of rare, toxic elements such as nickel and cobalt, which make them cost-effective and eco-friendly", adds Rana.

Different charging cycles under investigation

However, despite their attractive properties, Li-rich cathode materials suffer from certain drawbacks such as a reduction in battery voltage upon cycling known as the "voltage-fade" mechanism which reduces the energy density of a battery. In addition, there remains a fair amount of ambiguity especially about the role of the Li_2MnO_3 component in electrochemical processes of Li-rich materials, since it is believed to be electrochemically inactive. "The answers to these questions lie in thoroughly understanding electrochemical processes and associated structural changes in Li_2MnO_3", explains Rana.
The scientists investigated charged-discharged samples of Li_2MnO_3 during the first and 33rd cycles by X-ray absorption spectroscopy (XAS) using the synchrotron facilities of BESSY II at HZB and DORIS at DESY in Hamburg. They observed oxygen removal from the material during the first charge and shearing of oxygen layers as a result of the Li+-H+ exchange. These phenomena were previously proposed by various research groups. "The cumulative effect of such repetitive shearing of atomic layers during cycling is that the material gradually loses periodicity in atomic arrangements and, as a result, the electrochemical performance of a battery degrades upon cycling", claims Dr. Rana.
The observed structural changes in Li_2MnO_3 provide vital clues about the mechanism of electrochemical activation in Li-rich cathode materials. "A series of Li-rich cathode materials so far investigated by us show similar structural changes as observed in the case of Li_2MnO_3. Now that the electrochemical processes in Li-rich cathode materials are becoming clearer to us, we can use this knowledge to improve the cycling performance of these cathode materials", concludes Dr. Rana. *arö*

Adv. Energy Mater. 2014, 4, 1300998 (DOI: 10.1002/aenm.201300998): Structural Changes in Li_2MnO_3 Cathode Material for Li-Ion Batteries; J. Rana, M. Stan, R. Kloepsch, J. Li, G. Schumacher, E. Welter, I. Zizak, J. Banhart and M. Winter

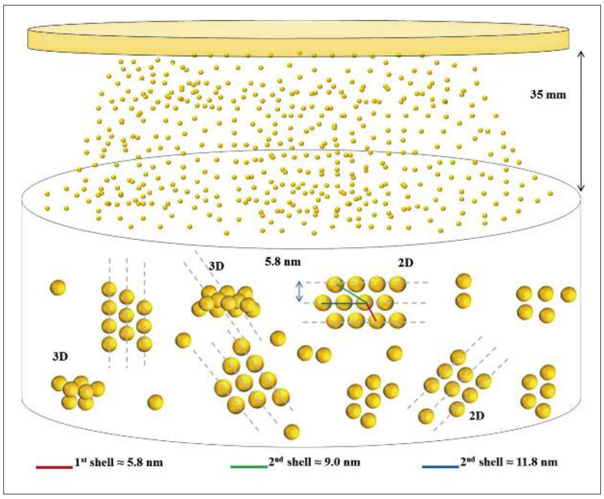
SELF-ASSEMBLY INTO CLUSTERS

Researchers of the HZB and Humboldt-Universität zu Berlin (HUB) used small-angle X-ray scattering at BESSY II to study the formation of **gold nanoparticles** in a solvent of vitamin B and urea. Their results are of great interest for catalysis research.

Prof. Klaus Rademann of the HUB and Dr. Armin Hoell of the HZB had not expected this result as they studied the formation of gold nanoparticles in a solvent. Instead of distributing evenly throughout the solution, the particles self-assembled into small clusters. They discovered this unusual behaviour while performing small-angle X-ray scattering at BESSY II. They subsequently confirmed their finding under the electron microscope. "What is special about the new process is that it is extremely simple and works with an environmentally friendly and inexpensive solvent", explains Klaus Rademann from HU Berlin. The formation of clusters is an important chemical process that can be used for technical applications in a targeted manner.
The solvent actually consists of two powders that one would sooner expect to find in agriculture than in a research laboratory: a supplement in chicken feed (choline chloride, aka vitamin B) and urea. British colleagues discovered a few years ago that mixing the two powders forms a transparent liquid able to dissolve metal oxides and heavy metals, called deep eutectic solvent (DES). The researchers in Berlin then positioned above the solvent gold foil that they could bombard with ions of noble gas in order to detach individual atoms of gold. This is how nanoparticles initially formed that distributed themselves in the solvent.

Nanoparticles stay small and form clusters

The longer the bombardment (sputtering) of the gold foil lasted, the larger the nanoparticles would become, the scientists reasoned. However, this was not the case: the particles ceased growing at five nanometres. Instead, an increasing number of nanoparticles formed over longer sputtering times. The second surprise: these nanoparticles did not distribute themselves uniformly in the liquid, but instead self-assembled into small groups or clusters that could consist of up to twelve nanoparticles.
These kinds of observations cannot be made easily under a microscope, of course, but require instead an indirect, statistical approach: "Using small-angle X-ray scattering at BESSY II, we were not only able to ascertain that the nanoparticles are all around five nanometres in diameter, but



Model of the self-assembly mechanism of clusters of gold nanoparticles.

also to measure what the separations between them are. From these measurements, we found the nanoparticles arrange themselves into clusters", explains Dr. Armin Hoell. "We ran computer models in advance of how the nanoparticles could distribute themselves in the solution to better understand the measurement results, and then compared the results of the simulation with the results of the small-angle X-ray scattering", explains Dr. Vikram Singh Raghuwanshi, who works as a postdoc at HU Berlin as well as HZB. An image from the cryogenic transmission electron microscope that colleagues at HU prepared confirmed their findings. "But we could not have achieved this result using only electron microscopy, since it can only display details and sections of the specimen", Hoell emphasises. "Small-angle X-ray scattering is indispensable for measuring general trends and averages."

Solvent is crucial

It is obvious to the researchers that the special DES solvent plays an important role in this self-organising process: various interactions between the ions of the solvent and the particles of gold result firstly in the nanoparticles reaching only a few thousand atoms in size, and secondly they mutually attract somewhat – but only weakly – so that the small clusters arise. “We know, however, that these kinds of small clusters of nanoparticles are especially effective as catalysts for the chemical reactions we want: a manyfold increase in the reaction speed due only to particle arrangement has already been demonstrated”, says Rademann. “The research on this phenomenon is now proceeding because we are convinced that such nanoclusters lend themselves as catalysts, whether in fuel cells, in photocatalytic water splitting, or for other important reactions in chemical engineering”, explains Hoell. *arö*

Langmuir, 2014, 30 (21), pp 6038–6046 (DOI: 10.1021/la500979p): Deep Eutectic Solvents for the Self-Assembly of Gold Nanoparticles: A SAXS, UV–Vis and TEM Investigation; V.S. Raghuwanshi et. al.

Chem. Commun., 2014, 50, 8693-8696 (DOI: 10.1039/C4CC02588A): Self-assembly of gold nanoparticles on deep eutectic solvent surfaces; V.S. Raghuwanshi, M. Ochmann, F. Polzer, A. Hoell and K. Rademann

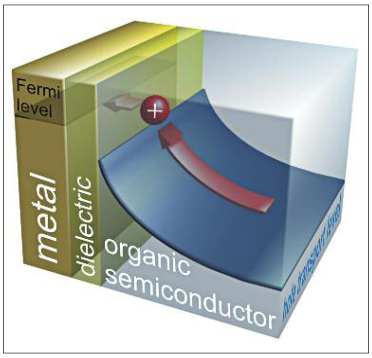
INSULATING LAYER IMPROVES ORGANIC SEMICONDUCTORS

HZB scientist Dr. Martin Oehzelt has developed a model that describes the behaviour of electrons at the interface between **organic semiconductors and adjacent metallic contacts**. His work contributes to the further improvement of these modern components.

Organic semiconductors allow for flexible displays, solar cells and other interesting applications. One common problem in these devices, however, is the interface between the metallic contacts and the organic semiconductor material, where undesirable losses occur. Currently, there are many different approaches describing the interface between organic semiconductor materials and metallic contacts. Oehzelt has unified them and developed a single coherent model based on the electrostatic potential caused by the charge carriers in the metal and the organic semiconductor.

The model shows what these losses between the metal and the organic semiconductors depend upon and how to minimize them. In particular, his model also explains why a thin, electrically insulating layer between the two materials can even facilitate the transition of charge carriers. “I calculated the impact of the charge carrier distribution on the electronic states at the interface and how these changes feed back onto the charge carrier distribution”, he explains. “It was surprising to me that the quantum physical level was not that important. The electrostatic effects predominated! The agreement between our model and the experimental data was astonishing.” On the example of pentacene, a common organic semiconductor, Oehzelt has quantitatively checked the model’s predictions for interface losses.

The energy distribution of the electronic states in organic semiconductors determines the minimum energy barrier the charge carriers have to overcome in transitioning from or into the metal. The calculation demonstrates that the shape of this energy barrier can vary, from a step-function to slow, continuously rising curves that lead to considerably lower losses. The latter can be achieved by introducing an extremely thin insulating layer between the organic semiconductor and the metal. Contrary to the general expectation, the introduction of an insulator thus improves the electrical contact. The results of this work could notably simplify optimization of interfaces and contacts and, thereby, the development of more efficient organic electronic devices. *arö*



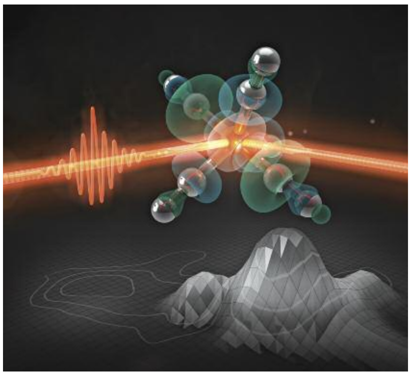
When inserting an ultrathin dielectric between metal electrode and organic semiconductor, charge carriers (shown here for a positively charged hole in red) are, counterintuitively, more efficiently extracted from their transport level (blue) in the organic to the Fermi level (black) in the metal than without the interlayer.

Nature Communications, 5, 4174 (DOI:10.1038/ncomms5174): Organic semiconductor density of states controls the energy level alignment at electrode interfaces; M. Oehzelt, N. Koch and G. Heimel

FEMTO-SNAPSHOTS OF REACTION KINETICS

An international team of researchers has decoded precisely how light affects the outer electrons of a metallic compound and activates it as a catalyst. This could be used to develop better **chemical storage devices for solar energy**.

All plants do it: they store solar energy in the form of carbohydrates with the help of a metallic compound. Chemically storing sunlight would also be ideal for society's energy needs. To develop this, however, we would need to better understand exactly what happens when photons strike molecules. The primary processes run on timescales of only a few hundred femtoseconds (one femtosecond = 10^{-15}s). An international collaboration led by Dr. Philippe Wernet has now been able to map the evolution of the chemical bonds in these kinds of ultrafast processes on the level of orbitals.
The team carried out their measurements on iron pentacarbonyl ($Fe(CO)_5$), a metal complex in which an iron atom is surrounded by five carbon monoxide groups. This yellow liquid is used as a primary material for synthesizing organometallic compounds and may also function as a catalyst. ($Fe(CO)_5$) has 18 valence electrons and is therefore inert like a noble gas, but can be activated by light. Photons cleave off a carbon monoxide so that the remaining $Fe(CO)_4$ molecule only has 16 valence electrons, making it a so-called 16-electron catalyst. Such homogeneous catalysts can be potentially used in converting methane to methanol, for example. $Fe(CO)_4$ is highly reactive, however, only as long as it is in the singlet state. If the molecule is instead in the triplet state, it remains inert and does not form further compounds. The experiment proved this law of quantum chemistry.



An ultrashort laser pulse activates iron pentacarbonyl as a catalyst. Scientists were able to observe the subsequent ultrafast processes experimentally by mapping the outer orbitals with an X-ray free-electron laser and interpret the obtained energy maps using quantum chemical calculations.

One year of set-up, but four years of evaluation

Twenty-one researchers from eleven research institutions participated in the research project – many of them within the Helmholtz Virtual Institute "Dynamic Pathways in Multidimensional Landscapes". Prof. Alexander Föhlisch and his team provided the unique expertise in time-resolved resonant inelastic X-ray scattering. The experiment was set up by the PhD student Kristjan Kunnus with Wernet and the team at HZB and in collaboration with Simone Techert and her group. After characterization at BESSY II, everything was shipped for 60 hours measurement to the X-ray free-electron laser LCLS of the SLAC National Accelerator Laboratory in the USA. It involves what is known as a pump-probe scheme in which a very short laser pulse in the optical region excites the valence electrons of the molecule (pump), while soft X-ray pulses arrive after a well-defined time delay in the femtosecond range later and probe the system for information. Michael Odelius' team and his PhD student Ida Josefsson at the University of Stockholm modelled the compound and its excited states using quantum calculations over the following years. Only after these calculations were made could the data be interpreted to such a level of detail that the experimental results could be unambiguously correlated with chemical interactions in the system. The results also show the extent to which the spin states of the electrons determine whether the molecules transition to reactive states or not after being excited by the sunlight. This is essential because actually both possible spin states in the present case were found to be represented due to the ultrafast transitions between singlet and triplet states. The measurements are a first step towards development of multidimensional X-ray spectroscopy in order to measure chemical dynamics on pulsed X-ray sources. "Now that we understand the reaction kinetics, we can control them or design a system to favour desired reactions, for example, in order to chemically store solar energy", says Wernet. *arö*

Nature, 520, 78-81 (DOI: 10.1038/nature14296): Orbital-specific mapping of the ligand exchange dynamics of $Fe(CO)_5$ in solution; P. Wernet et. al.

COMBUSTION OBSERVED ON A CATALYST

An international research team, with the involvement of the HZB, has observed for the first time the volatile intermediate stages that form at the exact moment when **carbon monoxide oxidises to carbon dioxide on a hot ruthenium surface**. The insights are important for developing higher performing catalysts – in motor vehicles, for example.

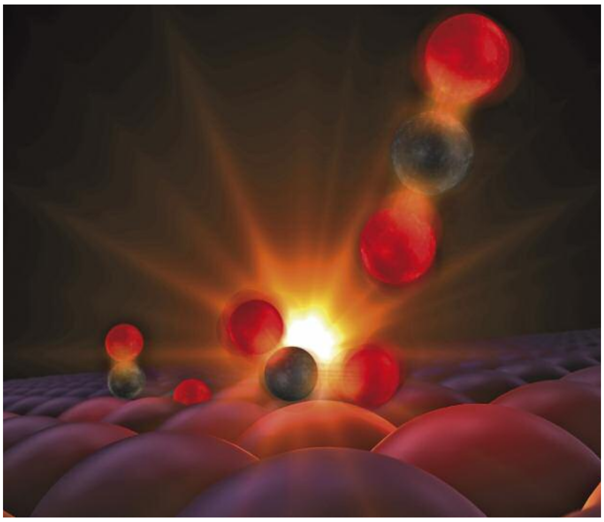
When molecules react together to form a new chemical bond, an energy barrier has to be overcome. It can be likened to rolling marbles up a hill: some of the marbles only make it part way up before rolling back down again without reacting with anything at the top. Other marbles make it all the way to the peak of the hill and enter a new state. Watching molecules at the exact moment when they overcome this energy barrier and form a new chemical bond – right at the peak of the hill – has long been considered impossible. “Because so few molecules are in this exact transition state at any given moment in a reaction, nobody expected we would ever be able to observe it,” says Prof. Anders Nilsson.

Yet this is exactly what Nilsson and colleagues managed to do – indeed during one of the most important chemical reactions of all, which is when toxic carbon monoxide bonds with oxygen to form carbon dioxide. The professor of the SLAC/Stanford SUNCAT Center for Interface Science and Catalysis and of Stockholm University led the research project. A team from the Institute of Methods and Instrumentation in Synchrotron Radiation Research from HZB has contributed to these research activities at SLAC sponsored by the Volkswagen-Foundation and the Helmholtz Virtual Institute “Dynamic Pathways in Multidimensional Landscapes” in which HZB and SLAC collaborate.

Only few stable CO_2 molecules

To study the reaction that takes place when toxic carbon monoxide is neutralised in the catalytic converter of a motor vehicle, the scientists used ultra-short X-ray pulses and laser pulses at the SLAC National Accelerator Laboratory, Menlo Park, California.

The reaction between carbon monoxide and adsorbed oxygen atoms was initiated by heating the ruthenium surface with optical laser pulses. Directly afterwards, changes in the electronic structure of oxygen atoms were probed via X-ray absorption spectroscopy as they formed bonds with the carbon atoms.The observed transition states are consistent with density functional theory and quantum oscillator models.

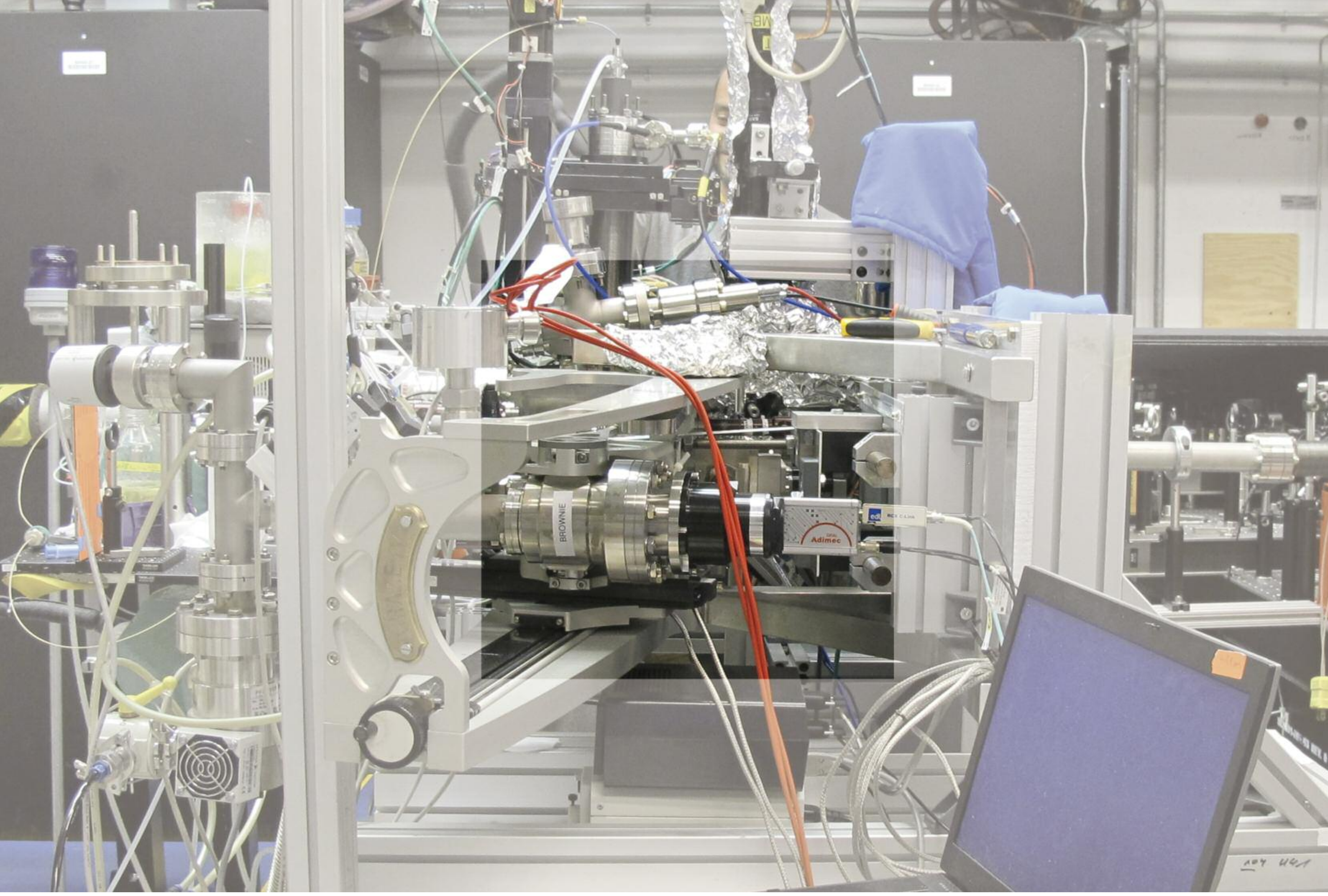


The image taken at SLAC illustrates a moment captured during the reaction of CO to CO_2, achieved for the first time.

The researchers were surprised to see so many of the reactants enter the transition state - and equally surprised to discover that only a small fraction of them go on to form stable carbon dioxide. “These results help us to understand a really crucial reaction with high relevance, for instance, for environmental issues and to see which role catalysts may play”, Martin Beye of the HZB Team explains.

The scientists had already investigated gas conversion in the catalytic converter in depth the previous year (see HZB Highlight Report 2013, page 31), and learnt how carbon monoxide molecules detach themselves (desorb) from a ruthenium surface. They discovered that weak bonds arose between the CO molecules and the catalyst surface. This and the new findings could help the automotive industry develop even more efficient catalytic converters for their future vehicles. *arö/SLAC*

Science, Vol. 347, 6225, pp. 978-982 (DOI: 10.1126/science.1261747): Probing the transition state region in catalytic CO oxidation on Ru; H. Öström et.al



FUTURE PROJECTS

Given that operation of the neutron source BER II set to finish in 2020, the Helmholtz-Zentrum Berlin is focussing its future activities on **energy and materials research, upgrading the photon source BESSY II and conducting research with photons**.

Positioned in the research fields **"Energy" and "Matter"** of the programme-oriented funding (POF) III programmes, the HZB is expanding its research activities on materials for energy conversion and storage and on energy-efficient components. Greater use will be made of the synchrotron radiation at BESSY II in these fields.

The new **energy materials research laboratory EMIL** has visibly taken further shape. Right on schedule, the building was ready to move into at the end of 2014, and installation of the scientific instruments is in full swing. After completion of the half-year commissioning phase in 2016, the laboratory is planned to go into full operation at the beginning of 2017.

With the **"Helmholtz Energy Materials Foundry (HEMF)"**, the HZB, as the coordinating centre, is planning a cross-centre Helmholtz research infrastructure and international user platform in the field of energy research. The application for this was submitted in 2014 and was recommended by the chairs of the scientific advisory boards.

DARK CURRENT IN THE LIGHT FROM BESSY II

So-called dark current interferes with the **generation of intense electron beams** as are required in linear accelerators such as BERLinPro. Dr. Roman Barday of the HZB Institute for Accelerator Physics and Dr. Stefan Lagotzky of the University of Wuppertal have developed a strategy for avoiding this effect.

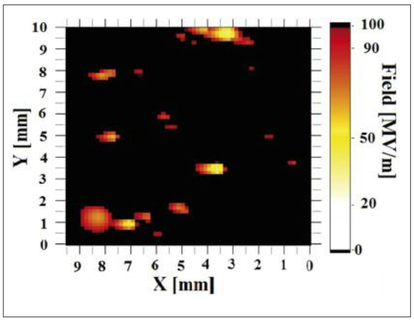
Electron beams can be used for many applications in physics research. Especially where high brilliancy and short pulse durations are needed, they are generated using a photocathode in a photo injector. The photocathode consists of an alkaline compound deposited on a molybdenum substrate. This is installed into a resonator and illuminated with short pulses of laser light. In the alkaline compound, the incident photons dislodge electrons, which are then emitted. An accelerator field accelerates the resulting electron beam up to high energy. Complications arise, however, when other mechanisms in the vicinity of the accelerator field also liberate electrons from the cathode material and substrate, and these electrons become accelerated as well. This unwanted "dark current" poses a high risk in the operation of the linear accelerator.

One important mechanism behind the generation of dark current is field emission, where the strong field of the accelerator's resonator allows the electrons to tunnel through the potential barriers between the photocathode material and the vacuum of the accelerator. Dr. Roman Barday and Dr. Stefan Lagotzky, working with scientists from two institutes at the HZB and Technical University of Dresden, studied the emission behaviour of monocrystalline and polycrystalline samples of molybdenum. The transition metal is often used for its favourable electronic properties as a substrate for high-efficiency photocathodes containing caesium or potassium, for example.

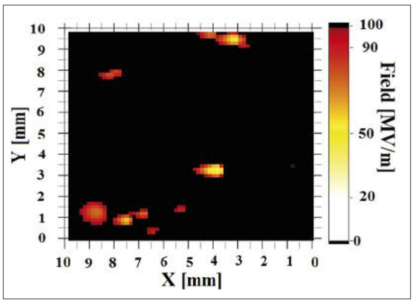
An oxide layer plays the key role

Using the field emission microscope (FEM) at the University of Wuppertal and employing X-ray photoelectron spectroscopy (XPS) at the synchrotron radiation source BESSY II of the HZB, the scientists analysed what measures can be taken to induce or avoid field emission. The FEM can make emission sources visible while XPS reveals their chemical composition. The researchers employed both experimental techniques on molybdenum samples under various electrical voltages and after different treatment methods. Prior to the experiments, they thermally treated the samples in the manner typical for producing molybdenum-based photocathodes: the material is heated to several hundred degrees Celsius in order to liberate gasses and separate off oxidised areas.

Yet, it appears this heating itself promotes the generation of dark current. The scientists namely found that an oxide layer that forms naturally on the smoothly polished metal surface prevents unwanted electron emission. If this is destroyed by baking in an oven at 400 degrees Celsius, then the probability of field-emission–induced dark current increases.



Field emission maps of an annealed oxide-free (top) and thermally oxidized Mo surface (bottom). The oxide apparently reduces the number of emitters providing 1 nA of current at fields of up to 100 MV/m.



The researchers furthermore revealed a way to avoid this dilemma: If the heating is done in a pure oxygen atmosphere, then the oxide layer remains intact even at high temperature. On the other hand, because the oxide layer impairs the function of the photocathode on the substrate, prior to preparation, it should be removed in a targeted manner by laser only in those places where the alkaline compound grows in the next step. This way, it should be possible to retain the desired emission behaviour of the cathode material while suppressing the unwanted emission of dark current.

rb

Eur. Phys. J. Appl. Phys., 2015, 70: 21301 (DOI: 10.1051/epjap/2015150167): Prevention of electron field emission from molybdenum substrates for photocathodes by the native oxide layer; S. Lagotzky, R. Barday, A. Jankowiak, T. Kamps, C. Klimm, J. Knobloch, G. Müller, B. Senkovskiy and F. Siewert

APPROACHING EMIL IN GREAT STRIDES

The HZB is coming close to completing its new laboratory EMIL. With this lab, the HZB experts are **creating worldwide unique opportunities** for studying materials for gaining renewable energy and for novel catalysts.

The Energy Materials In-situ Laboratory, EMIL, is a joint project of the Helmhotz-Zentrum Berlin and the Max Planck Association, and is being created as an annex to the synchrotron radiation source BESSY II. Since completion of the building extension in 2014, the hall has been filling with ever more high-tech equipment. "We are well on schedule, and can test the machines successively and get them ready for operation during the year," says Dr. Gerd Reichardt, the technical project manager for EMIL. The ultra-high vacuum transfer system, for example, was delivered in January 2015. With this system, material samples can be transferred from the chambers they were produced in to the analytical stations without interrupting the vacuum. The sensitive samples would be destroyed immediately in the normal atmosphere.

A cluster tool for the research on new classes of materials and device structures for photovoltaic and photocatalysis applications.

Two different undulators for brilliant soft and hard X-ray light

As a light source for EMIL, the HZB is building two new undulators, which will generate brilliant X-ray light over a particularly wide energy range, from soft X-ray light starting at 80 electron volts to hard X-ray light of up to 8 kiloelectron volts. "A single undulator could never cover such a broad spectrum. So we are building two very different types of undulators here," explains Dr. Johannes Bahrdt, who heads the undulator team. The soft wavelength range is served by an APPLE undulator, consisting of two lower and two upper series of differently polarised magnets. These series can be moved relative to each other so that even circular polarised light can be generated, which is of great utility in structural research. The actual challenge is the second undulator which will deliver the hard X-ray light. "Here, in collaboration with special companies, we are developing a so-called cryogenic undulator," Johannes Bahrdt tells us. The entire magnetic structure will be cooled with liquid nitrogen to around minus 200 degrees Celsius during operation, to guarantee sufficient stability of the magnetic material despite the very high magnetic field strengths.

A new cluster tool for EMIL to fabricate next-generation solar energy devices

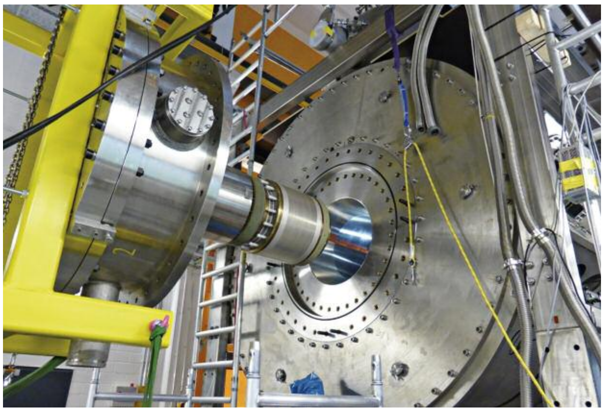
In order to research and develop materials for the next generation of high-efficiency solar cells at EMIL, HZB and Altatech, a subsidiary of Soitec, designed a new cluster tool. As part of the organizations' joint effort, Altatech has installed a new single-substrate multi-chamber solution, an AltaCVD system, at EMIL. The AltaCVD system can be used independently of the synchrotron to deposit amorphous silicon (alloys), transparent conductive oxides and ultra-thin dielectrics used in fabricating next-generation solar energy devices. The CVD system will be housed in the new EMIL building, adjacent to HZB´s third-generation storage ring BESSY II. The cluster tool is directly connected to a state-of-the-art X-ray analytical end-station, which accesses a dedicated beamline from BESSY II. "EMIL aims at exploring materials for high-efficiency photovoltaic cells and new catalytic processes for future solar energy generation and storage concepts," says Prof. Dr. Klaus Lips, head of the EMIL project and HZB´s Advanced Analytics Group.
EMIL is planned to be connected to the synchrotron light of BESSY II in the autumn of 2015. "It will be a very special moment when we connect the EMIL beamline to the storage ring," Klaus Lips declares. "Then, EMIL will be armed and the research can begin."

hs/arö

HIGH-FIELD MAGNET EXCEEDS EVERYONE'S EXPECTATIONS

The new high-field magnet of the HZB is consistently producing magnetic fields of **approximately 26 tesla** and staying at this value over extended periods of time. In the spring of 2015, after eight years of building and development, it was put into the service of science.

With high expectations, HZB scientists and researchers from around the world have waited for the new high-field magnet at HZB, that was developed at the National High Magnetic Field Laboratory (NHMFL) in Tallahassee, Florida, USA. Certain quantum physical phenomena in matter can only be clearly visualized in the presence of extreme magnetic fields and, in many cases, neutrons are the ideal probes to use. This combination of high magnetic fields and neutrons is offered only by the HZB. In the presence of these extreme, 20-tesla



Insertion of the resistive Bitter coil into the superconducting coil. These strong copper lines provide current.

and greater magnetic fields, new order states and phase transitions in high-temperature superconductors, new IT materials, and other samples can now be experimentally investigated for the first time ever.
The first implementation of the HZB´s high field magnet went comparatively smoothly. "We were able to address most of the issues which arose during testing really quickly," says project coordinator Dr. Hartmut Ehmler. This shows that quality control measurements during production of the coils and the set-up of the magnet system worked well.

All systems thoroughly tested

A separate test of the resistive coils was already performed after completion of final assembly in June 2014. After cooling the superconducting coils, which took several weeks to complete due to their enormous mass, the crucial tests of the hybrid system with both coils in series connection were able to be performed in mid-August: ramping up power from zero to only 1,000 amperes and greater. In the process, the team tested how the system would respond to changes in current intensity (induction), which forces and voltage spikes occurred in the process, and whether or not this was consistent with previous calculations of the magnet's performance.
For security reasons, performance of the whole facility during an emergency shutdown and other incidents were tested. Until the very end, everyone was on edge to see whether or not the last several thousand amperes would bring any surprises before the finish-line could be crossed. Luckily, all systems cooperated without incident, so that the current could be incrementally increased up to a final value of 20,000 amperes.
Having passed its tests at the end of December 2014, the high-field magnet was relocated to its final installation site in the neutron guide hall at BER II. There, it had to be connected once again to its supply lines for water, helium and electricity. Finally, in the beginning of May, it was officially put into operation. *hs/arö*

NEAT II MAKES PROGRESS

Construction of the new time-of-flight spectrometer NEAT II at the neutron source BER II made further progress last year. In September 2014, the detector chamber constructed in Spain was delivered and built into the extension made specially for the instrument. Inside the chamber, it is measured how long the neutrons take to travel from the sample to the detector that catches them. So indeed, true to the name of the method, the actual time of flight of the neutrons is measured. "By the end of 2015, all parts of the time-of-flight spectrometer should be installed, so that we can commence user operation some time during 2016," says Dr. Margarita Russina, who is managing the project at the HZB.

SUCCESS MODEL "JOINT LABS"

With now ten "joint laboratories" the HZB is an important driver for networking within the **scientific region of Berlin/Brandenburg**.

Opening: The "Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE)" founded jointly by the HZB, Freie Universität Berlin and the Zuse Institute Berlin, went into operation in February 2015.

Over recent years, the HZB has established several "joint laboratories" with universities and institutes to create a solid foundation for collaborative efforts. With each lab associated with a junior professorship, the model ensures that select experts not only research at the HZB, but are also involved in teaching at the universities. The newest joint lab, founded in February 2015 by the HZB, Freie Universität Berlin and the Zuse Institute Berlin, is the "Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE)". Its purpose is to research and develop materials for photocatalysis, photovoltaics and photonics with structuring at the nanometre scale. An important focus is the 3D simulation of individual components and of whole functional systems.
The experience gained from the joint labs so far shows that this type of cooperation is highly advantageous for both the HZB and the university partners – all resources are being used with maximum efficiency and scientific productivity is increasing. At the same time, the attractive power of Berlin as a location is increasing for young scientists, and promotion of young talent is becoming an important pillar in the HZB profile. In the scope of the Excellence Initiative as well, the joint labs could one day serve as a model for the better networking of university and non-university research. Currently, there are nine joint labs in the Berlin-Brandenburg region, and one with the University of Uppsala in Sweden. Here is an overview of the joint labs and the corresponding partners:

- **Joint Lab for Structural Research (JLSR)** with HU Berlin and TU Berlin
- **Joint MX Lab** with HU Berlin, MDC, FU Berlin and Leibniz-Institut für Molekulare Pharmakologie (FMP)
- **Joint Lab on Accelerator Physics (JLAP)** with HU Berlin
- **Berlin Joint EPR Lab (BeJEL)** with FU Berlin
- **Berlin Joint Lab for Supramolecular Polymer Systems (BerSuPol)** with FU Berlin
- **Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE)** with FU Berlin and Zuse Institute Berlin (ZIB)
- **Joint Ultrafast Dynamics Lab in Solutions and at Interfaces (JULiq)** with FU Berlin
- **Berlin Joint Lab for Non Equilibrium of Matter (BerNEM)** with FU Berlin
- **Berlin Joint Lab for Quantum Magnetism (BerQuam)** with FU Berlin
- **Uppsala Berlin Joint Lab (UBjL)** with the University of Uppsala

RESEARCH INTO NOVEL ENERGY STORES

At the beginning of 2015, the Helmholtz Association created the research programme "Storage and cross-linked infrastructures". Five Helmholtz centres are researching into cross-system technologies that can balance out power fluctuations, and are developing infrastructures in which different energy carriers can be interconnected. The programme has a 5-year budget of around 310 million euros and is divided into six topics: batteries and electrochemical stores, electrolysis and hydrogen, synthetic hydrocarbons, fuel cells, thermal energy stores, and grids and storage integration. The HZB is covering the topic of batteries and electrochemical stores, including the development of storage solutions through to the application stage.

JUBILEE FOR CHARITÉ AND HZB

IN NOVEMBER 2014, THE **2,500th EYE TUMOUR PATIENT** RECEIVED SUCCESSFUL PROTON TREATMENT.

Patient in the treatment chair before the use of the photon beam.

Numbering at around 500 to 600 new cases each year, choroidal melanoma is one of the rarer diseases in Germany. The Charité Eye Clinic on the Benjamin Franklin Campus is specialised in treating this very rare tumour disease. Since 1998, Charité has treated more than 200 patients from across Germany and other European countries, such as Austria, Poland, Bulgaria and Serbia, with proton beams at the HZB. Given the intricate nature of the eye, proton therapy for choroidal melanoma is only performed at twelve centres in the world. In Germany, the HZB is the only location where such treatment is possible.
The HZB group led by Dr. Andrea Denker assures the quality and precision of the proton beam and makes continual advancements to the methods for beam diagnosis and dosimetry. “We can use accelerators that were once used for basic research. With the cyclotron and its pre-accelerators, we have a system that is capable of producing a proton beam with the ideal energy, intensity and time structure for eye tumour therapy,” she says. More than 95 percent of patients treated are tumour-free after five years. Depending on the location of the tumour, useful vision can be maintained in most cases.

HANDS-ON PHYSICS

FOR TEN YEARS, THE HZB HAS RUN A **SCHOOL LAB**, VISITED EVERY YEAR BY MORE THAN 2,000 CHILDREN AND ADOLESCENTS.

The two HZB School Labs are dedicated to subjects such as “light and colour” or “solar energy”.

The HZB’s School Lab started out by raising schoolchildren’s awareness of how attractive a scientific career can be – over the years, for many schools it has since become a natural supplement to classes. At first, pupils from the higher grades of strongly scientific grammar schools would come to do experiments on electromagnetism and superconductivity. Now, the School Lab is in especially high demand among the 5th and 6th grades who are just taking their first science classes. “The kids get to see that physics isn’t just a subject they have to swot at school, but is actually the basis for working in research centres,” says Michael Tovar, who headed the School Lab in Wannsee up until the summer of 2015, when he returned to his own research.
Together with teachers, Michael Tovar and Ulrike Witte, head of the second School Lab established in Adlershof in 2010, have developed multiple series of experiments that reflect the research being done at the centre, and which are simultaneously oriented along the school curricula. In workgroups, curious school kids can put their own experimental ideas into practice, and even take part in “youth research” projects. The HZB School Lab also organises the annual Girls’ Day at the HZB, and provides experimental stands for the Long Night of Science and other events.

EXCELLENT COMMUNICATION

SINCE THE BEGINNING OF 2014, THE HZB HAS KEPT ITS INTERESTED PUBLIC UP TO DATE ON ITS FUTURE PROJECTS WITH THE **#HZBZLOG**, FOR WHICH IT HAS ALREADY RECEIVED AN AWARD.

In January 2014, the HZB opened a new interactive window into science with the #HZBzlog. Unlike classic scientific communication channels, there is no focus on finished results here, but instead a direct experience of what science is achieving right now. The #HZBzlog is a mixture between a group blog, a magazine and a long-term documentary. The topics covered are the future projects of the HZB, including high-field the magnet, BESSY-VSR and EMIL.
Just a few months after it was launched, the new format was distinguished with the German Online Communication Award from the Deutsche Presseakademie (German Press Academy). “We are delighted by this award, because it means we managed to impress the assembled experts in the field of corporate communication with our project,” says Ina Helms, head of the communications department of the HZB. “And we are delighted, above all, that our prominent figures in science are so actively involved.” The site attracts as many as 1,000 users daily.

ANTS FINKE IS THE NEW HEAD OF IT

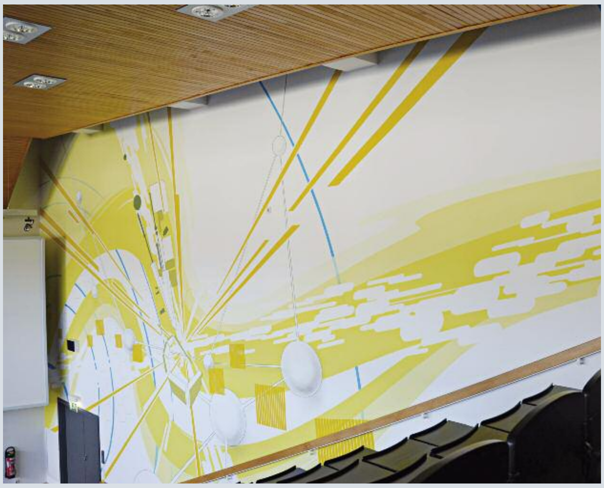
SINCE OCTOBER 2014, FINKE HAS HEADED THE RECENTLY FOUNDED **HZB INFORMATION TECHNOLOGY DEPARTMENT.**

When he came to the HZB, the 50-year-old mathematician was responsible for the software division of the data processing centre of the state of Mecklenburg-Western Pomerania. Since the spring of 2015, at Finke’s suggestion, the IT Department has been structured into four divisions: IT-IS (Infrastructure), IT-DS (Services and Software), IT-FH (Front Office and Helpdesk) and IT-ED (Experiment Control and Data Acquisition). These departments are complemented by an Office for Interdivisional Tasks responsible for introducing operational processes. “This new structure helps us to assign duties according to the exact field of activities, and to effectively handle all of the tasks that come our way,” Finke says. “Another complex issue is how research data will be handled in future. A data policy should create the necessary rules for handling the data, where the IT Department will offer the technical framework based on that,” he explains.

ERNST-ECKARD-KOCH PRIZE FOR DR. MARKUS RIES

In December 2014, the Friends of HZB awarded for the 24th time the Ernst-Eckhard-Koch Prize for outstanding promotional work in the field of research with synchrotron radiation. Accelerator physicist Dr. Markus Ries (pictured on the left together with Prof. Mathias Richter) received the prize for his work on “Nonlinear Momentum Compaction and Coherent Synchrotron Radiation at the Metrology Light Source” at HU Berlin. His results flow directly into the future project BESSY-VSR of the HZB, in which Markus Ries continued his research as a postdoc. Dr. Alex Manuel Frano Pereira (pictured on the right), now a postdoc at the University of California Berkeley, was also awarded the prize for his promotional work.

GRAFFITI IN THE AUDITORIUM



The artists Gerrit Peters and Heiko Zahlmann redecorated the auditorium in Wannsee in the spring of 2014. With their paint rollers, brushes and spray cans, and helped by two art students, they spent eight days applying the motif on the large wall in the auditorium: Their theme artfully represents wave-particle duality as a common denominator in research, as well as various topics researched at the HZB. The design by the artist team from Hamburg was approved in a competition held by the HZB.

PROF. DR. SEBASTIAN SEIFFERT TWICE DISTINGUISHED

In the spring of 2014, Prof. Sebastian Seiffert, who heads a workgroup at the "Institute of Soft Matter and Functional Materials" at the HZB, was presented the Annual Award of the Association of German University Professors in Chemistry (ADUC). Seiffert (pictured on the right) was handed the award by Prof. Roland Winter during the Conference of University Professors of Chemistry at TU Paderborn. In the summer, Seiffert also received the award for junior scientists in the field of macromolecular chemistry from the German Chemical Society (GDCh). Seiffert and his group study switchable microgel particles for use in many different applications. He is especially interested in how the behaviour of these materials depends on their nano-architecture.

NERNST-HABER-BODENSTEIN PRIZE FOR PROF. DR. EMAD AZIZ

In May 2014, the German Bunsen Society for Physical Chemistry presented Prof. Emad Flear Aziz with the Nernst-Haber-Bodenstein Prize. Aziz heads his own workgroups at the HZB and at Freie Universität Berlin, and is establishing the joint laboratory JULiq (Joint Ultrafast Dynamics Lab in Solutions and at Interfaces). Aziz develops new methods for studying the structure and dynamics of ultrafast processes and phenomena in solutions and at interfaces.

IMPORTANT APPOINTMENTS

Prof. Dr. Sebastian Seiffert assumed a W2 professorship of "Supramolecular Polymer Materials" in April 2014 which is jointly funded by the HZB and Freie Universität Berlin.

Prof. Dr. Silke Christiansen received a three-year honorary professorship at the Faculty of Semiconductor Physics and Chemistry of the South Korean Chonbuk National University in May 2014.

Prof. Dr. Christiane Becker took over a professorship at the Berlin University of Applied Sciences (HTW Berlin) in the winter semester of 2014, where she teaches in the department "Engineering Sciences – Energy and Information".

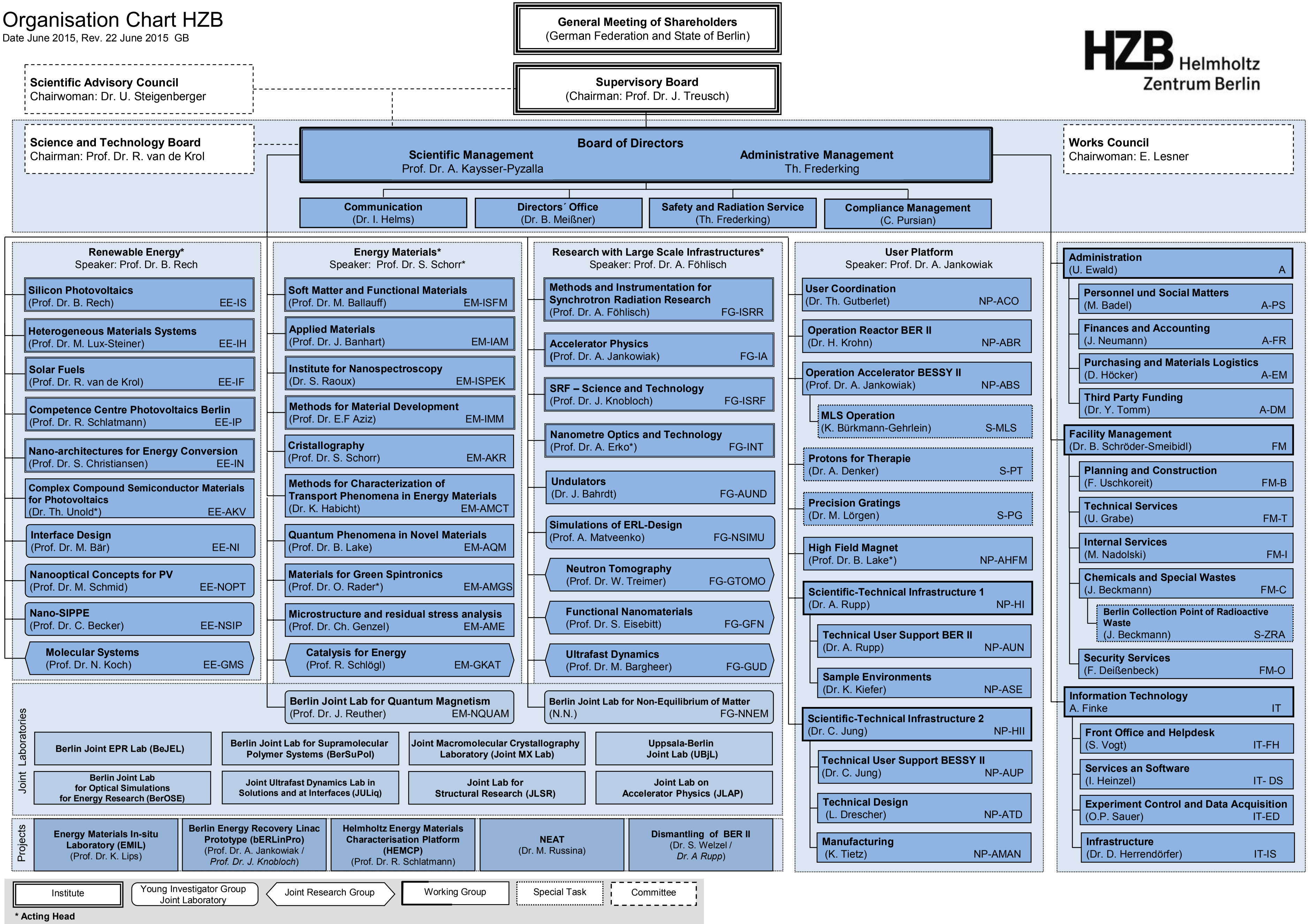
Prof. Dr. Christiane Stephan has been appointed a junior professor of "Technical Mineralogy and Energy Materials" at FU Berlin.

Prof. Dr. Johannes Reuther was appointed a junior professor with FU Berlin in the scope of the Berlin Joint Lab for Quantum Magnetism (BerQuam) in August 2014.

Dr. Simone Raoux has been the Head of the Institute of Nanospectroscopy at the HZB since January 2014. She was recruited through the Helmholtz Recruiting Initiative of IBM. Appointment proceedings are underway for an S-W3 professorship with HU Berlin.

Organisation Chart HZB

Date June 2015, Rev. 22 June 2015 GB



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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