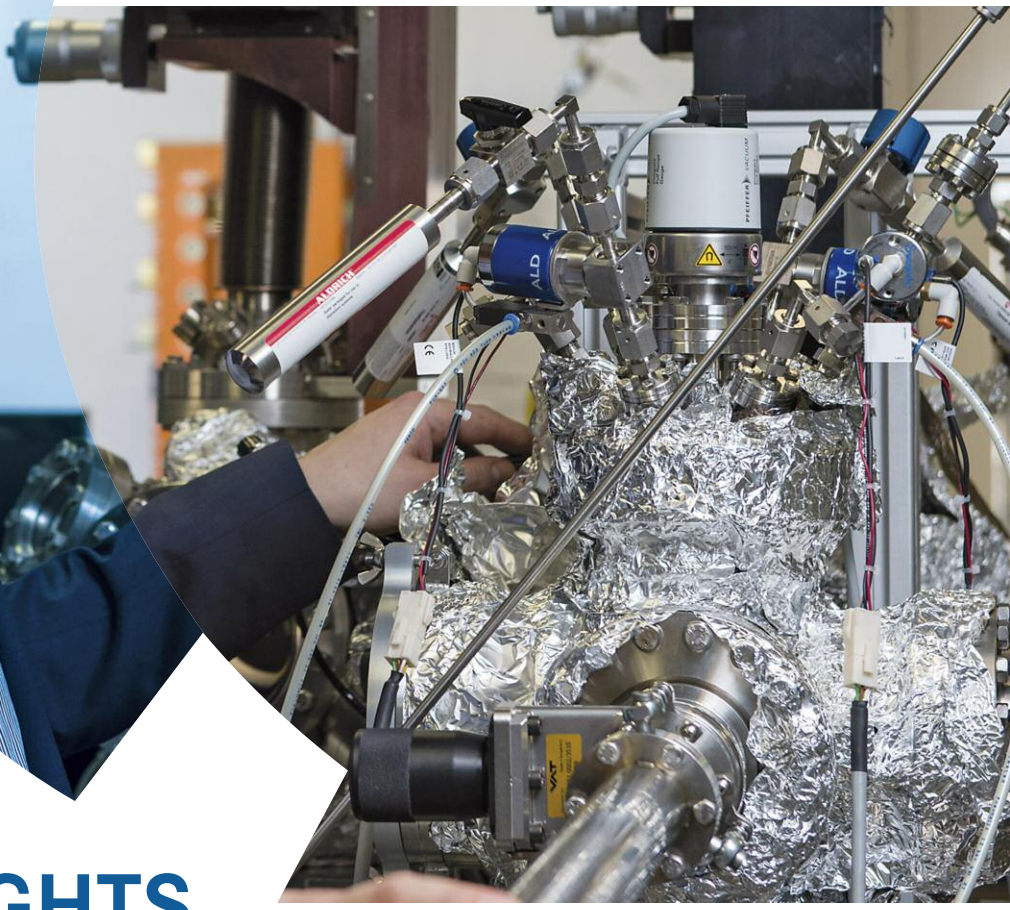
HZB Helmholtz Zentrum Berlin

FOCUSSING ENERGY REALISING VISIONS



HIGHLIGHTS 2013

Annual report with research highlights at the

Helmholtz-Zentrum Berlin für Materialien und Energie

CONTENTS

A YEAR OF STRATEGIC ALIGNMENT

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

The year 2013 was a special one for the Helmholtz Centre Berlin for Materials and Energy. We were able to look back on the first five years of our existence after the fusion of the Hahn-Meitner Institute and BESSY – and thus at the same time on the first joint period of sponsorship within the framework of the Helmholtz-wide programme-oriented sponsorship (POF). The current sponsorship period (POF II) will expire in 2014. We have worked intensively over the past months to prepare for the next POF period (POF III), which starts in 2015. Our international experts took a critical look at all of the programmes in the spring of 2014 and posed these questions: Have the structural changes had the desired effect? Can the new programmes make a significant contribution to solving the enormous challenges that confront us – for example, sustainable energy supplies, materials for the computer technology of the next generation or mobility of the future? And how does HZB stand in comparison with the other Helmholtz centres? Is our joint venture with them and other partners, for example the universities, on a good basis? We will receive the answers to these questions in writing during the course of 2014.

> "The decision to operate our neutron source BER II for only one more sponsorship period, in other words until the beginning of 2020, was far from easy. But it provides HZB with the possibility of changing its strategic focus and to occupy new and scientifically promising research fields with respect to energy and materials."

Although we still have to be patient a while longer, we would already now like to sincerely thank all those who participated in this appraisal. Our staff worked very hard and made great efforts to present HZB in its best light. Over a long period that extended into the first six months of 2014, they performed excellently in all phases of the appraisal. To start off with, they showed huge dedication in refining and polishing the programme applications, fine-tuning the strategies thereby with which we want to further our science. And then, when it came to the on-site presentations, the entire HZB team displayed perfect organisation. We were able to create a fantastic atmosphere for the experts and heard many original presentations that allow us to look forward to the coming years with great enthusiasm and confidence. This is all the more remarkable because for the first time, we have made a leap from involvement in two Helmholtz programmes to six programmes in which the HZB participates.

The most far-reaching strategic decision during this period was without doubt the decision to operate our neutron source BER II for only one more sponsorship period, in other words until the beginning of 2020. This decision was far from easy, but it provides HZB with the possibility of changing its strategic focus. The early announcement of our plan also makes it possible for us to occupy new and scientifically promising research fields with respect to energy and materials. The research especially into new sustainable energy production concepts has gained enormous momentum. This is testified to by the excellent appointments on offer, newly established institutes and departments as well as the ongoing development of the Energy Materials In-Situ Laboratory Berlin (EMIL). At the same time, we will be focusing our large-scale facilities on the research with photons from 2020 onwards.

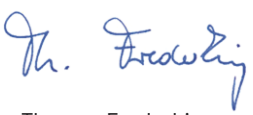
This fine-tuned profile and the unique expertise we have built up on the sector of accelerator physics will give us a competitive edge when applying for large-scale expansion investments. And the way in which the BESSY-VSR project is developing demonstrates clearly that our chances here are very good. The concept of developing an accelerator which generates variable light pulses, i.e. short and long pulses in one ring, from the existing BESSY II storage ring has already succeeded in convincing many experts.

HZB is also adopting new approaches in the communication of such projects. Those interested can now go on-line in our "logbook of everyday science", the #HZBzlog, and follow quasi live exactly how projects and infrastructures currently under development are taking shape and exactly what tasks the scientists and engineers are confronted with every day. Whereas the #HZBzlog permits you to take an exclusive peek over the shoulders of our scientists and thus offers an open window showcasing our current activities, this Highlight Report is intended in the traditional manner to present selected research work which has been published and thus successfully concluded. This report details in the customary way successful user experiments and experiments from our own research.

"With a fine-tuned profile and the unique expertise we have built up on the sector of accelerator physics will give us a competitive edge when applying for large-scale expansion investments. And the way in which the BESSY-VSR project is developing demonstrates clearly that our chances here are very good."

In other words, you will on the one hand find the structure you are accustomed to in this Highlight Report, but on the other hand, there is also something special. Occasioned by HZB's fifth anniversary, namely a removable poster with which you can trace the development of HZB in a timeline. We have focused on topics which are of overriding importance for HZB, for example the promotion of young investigators and the cooperation with universities. Besides this, we have selected projects which show that the HZB is more than just the sum of its former parts, i.e. the Hahn-Meitner Institute and BESSY GmbH. Projects such as EMIL, which neither of the former centres could have developed alone. We hope you like the enclosed poster and that as a reader, will continue to follow the development of HZB with interest. As always we hope you enjoy reading our report and why not pay us a visit on www.hzbzlog.com sometime?

Prof. Dr. A. Kaysser-Pyzalla
Scientific Director



Thomas Frederking
Administrative Director

A TIME FOR AMBITIOUS GOALS

The sun radiates more than enough energy onto the earth to supply the entire human race with energy. However, in order to cover the demand, the possibility of storing solar energy is essential, for example in the form of hydrogen. HZB was able in 2013 to announce a first breakthrough with a robust system made of reasonably priced components. We talked to **Professor Dr. Roel van de Krol** about the development of this research field and the objectives that HZB is pursuing thereby.

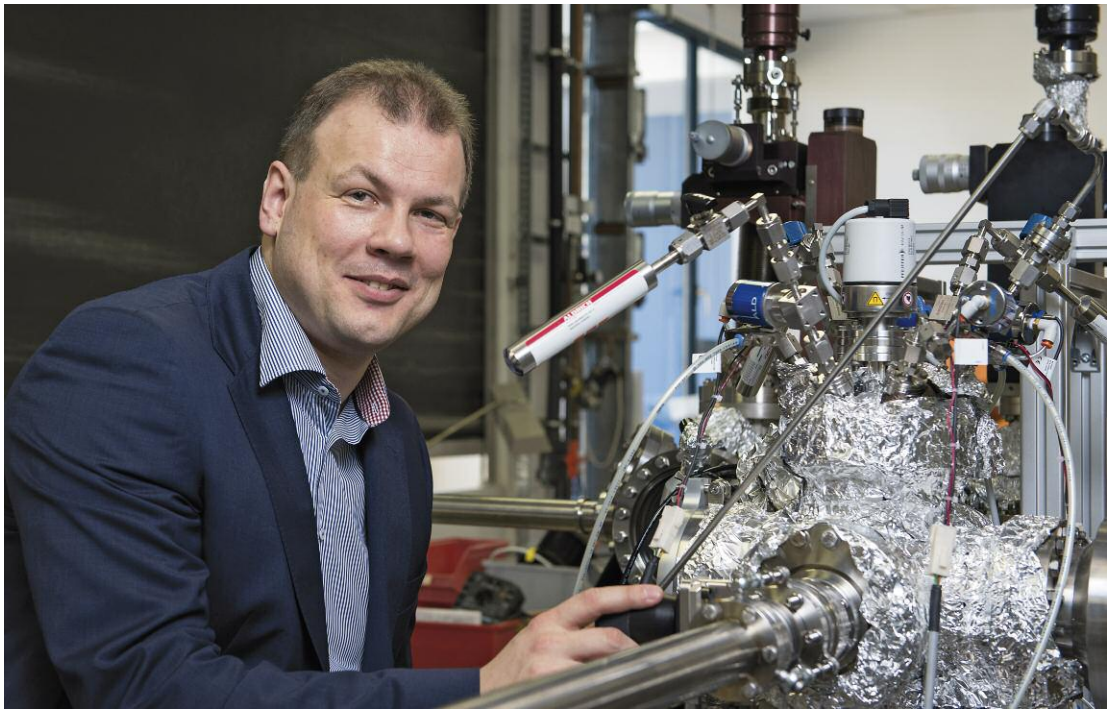
Mr van de Krol, you have headed up the HZB Institute for Solar Fuels for a year now. Since when have teams of researchers actually been working on solutions for the production of solar hydrogen?
It all started in 1972 when Japanese researchers demonstrated that water with a semiconducting oxide can be split into hydrogen and oxygen. Because of the oil crisis in 1973, there was enormous interest at first in generating hydrogen from sunlight as an alternative to fossil fuels. However, from the 1980s onwards, interest dwindled and it was merely a handful of groups that persevered with this research. But since about five years, this research field has once again become a really hot topic. This is naturally a direct result of the climate change and the energy turnaround. We need affordable and efficient solutions for storing solar energy, and hydrogen production is an extremely good option. At the same time a great deal of progress was made which makes this option much more realistic. For example, Michael Graetzel from Lausanne showed in 2006 that nanostructured iron oxide permits the generation of extremely good photocurrents, which is basically rust, and therefore a correspondingly cheap material.

In summer 2013, you were able together with the TU Delft to announce a breakthrough. What was it exactly?
We built a relatively simple system that achieves five percent efficiency and good stability. We use a conventional thin-film silicon cell and combine this with a metal oxide. This has two advantages: on the one hand, the metal oxide converts yet another part of the light spectrum into electric current, and on the other hand, it protects the sensitive silicon cell against corrosion. You might say we are combining the best of two worlds. We received a lot of attention, also from the media, which goes to show just how great the interest in storage solutions for renewable energy is.

Such systems are often called “synthetic leaf systems” because they use sunlight in the same way as plants do in order to split the water. How does this differ from biological systems?
At about one percent, the efficiency of photosynthesis is very poor, but nature naturally has objectives other than maximum efficiency. In contrast, synthetic systems could theoretically reach an efficiency of between 25 and 30 percent. As early as 2001, scientists built a system that was capable of chemically storing around 18 percent of the sunlight. The system, however, was made up of at least 16 layers and was extremely expensive. In order to develop a practicable and marketable system, we not only need to increase the efficiency, but also to improve the stability and simultaneously reduce the costs. Besides this, it must be possible to produce these systems on a large scale. The challenge is to find the best compromise between these requirements.

HZB COORDINATES PECDEMO

In a mere three years, the research partners of the EU project PECDEMO want to develop a compact system that is suitable for practical application and that converts at least ten percent of solar energy into hydrogen. They also want to produce a large-scale module of 50 square centimetres intended to achieve a conversion efficiency of at least eight percent and which remains stable for over 1,000 hours. That could just constitute the breakthrough for practical applications. Prof. Dr. Roel van de Krol coordinates the international research project and has taken renowned partners on board: PVcomB and DLR, the group working with Michael Graetzel from the École Polytechnique Fédérale de Lausanne, Switzerland, the Israel Institute of Technology in Haifa, Israel, and the University of Portugal. The industrial partners are EVONIK Industries and Solarnix SA. Over the three years of its term, PECDEMO will be funded with 1.83 million euros, 440,000 euros of which will go to HZB.



Prof. Dr. Roel van de Krol, head of the Institute for Solar Fuels at HZB.

What are the major unsolved questions and which ones do you want to tackle?
I believe that as far as solar fuels go, we are currently there where photovoltaics was 40 years ago. Our greatest challenge will be to find the ideal, magic material, just as silicon is for solar cells. The material must be an extremely good light absorber, must remain chemically stable and must not be too expensive. I hope that we will be able to develop one or two such really new materials over the next five to ten years. At the same time, we are not exactly sure of how defects develop and what role they play for the efficiency of the system. We plan to systematically investigate this question with a great number of different metal oxides. And we naturally keep an eye on what the others are doing and then pursue our own approach. The Americans, for example, start off with extremely good solar cells and then try to make them more stable against corrosion. We on the other hand start off with cheap and robust materials such as the metal oxides and then try to increase their efficiency.

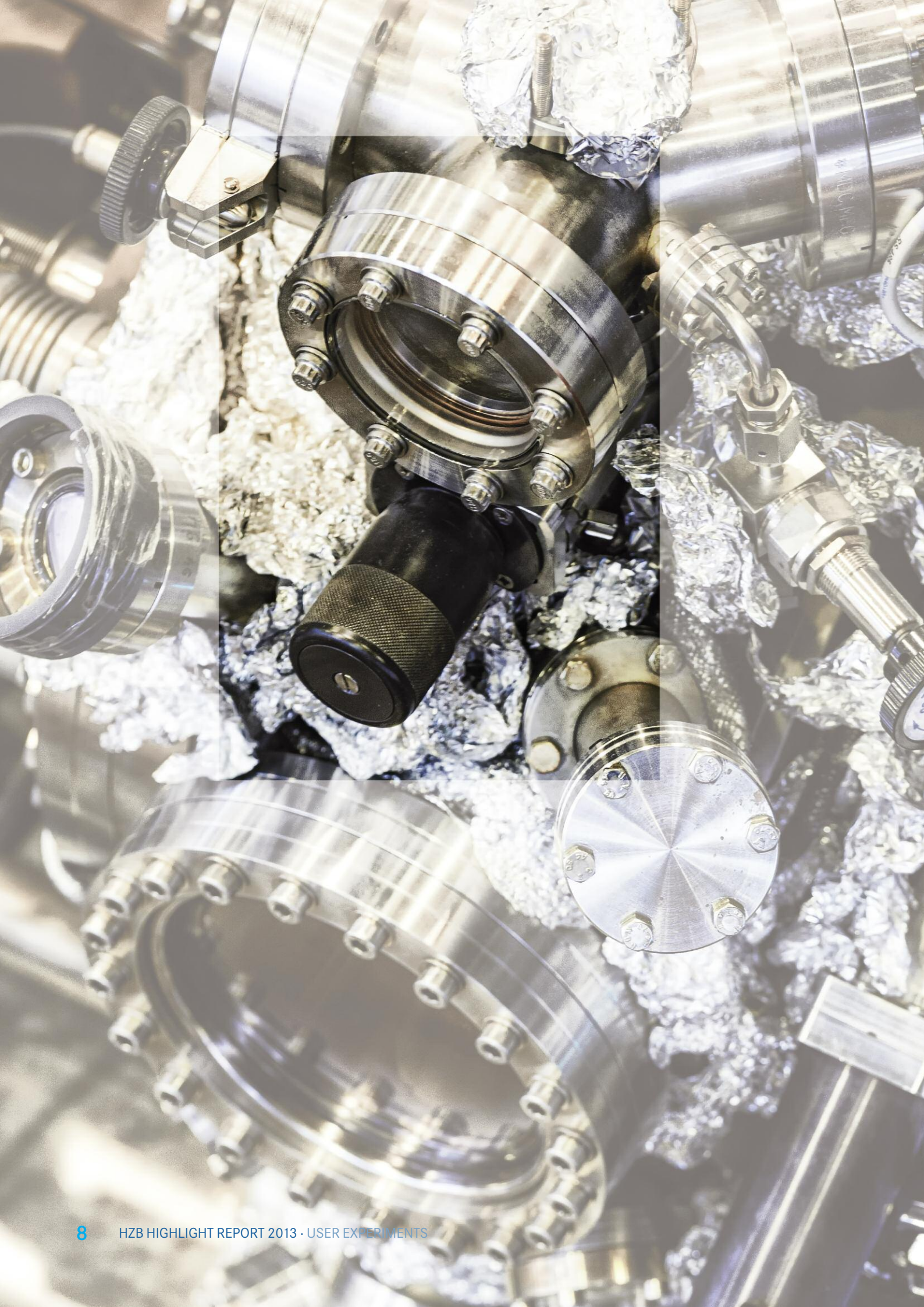
Where is HZB on an international level?
With their EnergyHub programme, the USA have injected tremendous impetus into research. The Joint Center for Artificial Photosynthesis (JCAP) at CalTech in California, with whom we also work, is the largest initiative on the entire planet for solar fuels; and Brazil, Korea and Sweden also have their own research centres for artificial photosynthesis. With its Institute for Solar Fuels, HZB constitutes one of the larger groups in Europe. We are a team of around 50, but that is naturally not what counts: with EMIL, we will be able to produce hundreds of samples with slight variations in their composition and simultaneously to characterise them. That is what sets us apart from others and gives us a competitive edge.

What are your specific objectives for the next few years?
As a Helmholtz Centre, we also have the mandate of going beyond the realms of basic research and demonstrating that such systems are feasible. In April 2014, we at HZB started the EU project PECDEMO in the capacity of coordinators. In the next three years, we want to develop a system that can store at least eight percent of solar energy and which thereby remains stable for a thousand hours. That is a magical number in order to win over the industry for the technology. Setting such clear goals is naturally risky, but we want to take the risk. We have been talking about this technology since the 1970s, and it has progressed in leaps and bounds over the last five years. We feel we are now in a position to set ambitious objectives.

Antonia Rötger conducted the interview

SUMMARY

- The ability to store solar energy in the form of hydrogen is considered the key to realising an eco-friendly energy supply.
- In 2013, researchers from HZB and the TU Delft succeeded in building a simple and stable system capable of converting 5 percent of solar energy into hydrogen.
- In theory, it would be possible to store up to 30 percent of solar energy.
- HZB and its partners have set their sights over the next three years on a system that can store 8 percent of solar energy and which remains stable for at least 1,000 hours.



HIGHLIGHTS FROM USER EXPERIMENTS

More than 3,400 user visits to the electron storage ring BESSY II in Berlin-Adlershof were recorded in 2013, working in nearly 400 research groups from 31 countries.

Over 7,000 operating hours went into scientific use of the storage ring facility BESSY II in the past year. Subtracting the time for accelerator experiments and factoring in the availability of individual beamlines and experimental stations, this equates to approximately 12,000 eight-hour shifts worked by visiting experimenters on 38 beamlines and experimental stations.

Around 84 percent of the available shifts were used by scientists for their research: Some 70 Percent were used for external scientific projects; HZB in-house scientists used further 14 percent of measurement time for their own research. Technical downtimes and training accounted for roughly 16 percent.

171.5 days with eleven reactor cycles was how long the neutron source BER II in Berlin-Wannsee was in operation last year. 15 instruments amounting to over 2,500 instrument days were available during this period. Of these, the scientists required nearly 430 days for maintenance and instrumentation. Researchers spent more than 2,000 instrument days on their experiments.

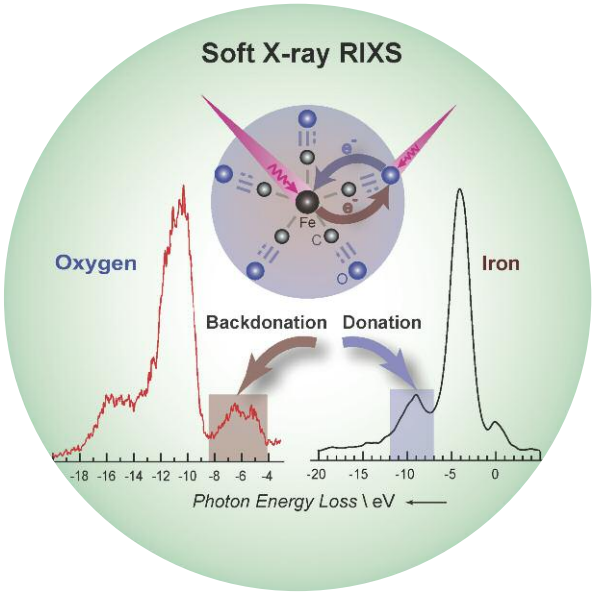
Around 61 percent of the available measurement time at BER II was used by external visiting experimenters for short-term projects and nearly 12 percent for long-term projects. HZB scientists used approximately 560 instrument days (around 27 percent), for in-house research.

248 projects were awarded measurement time at BER II in 2013 – that equates to 75 percent of all projects for which beamtime applications were submitted. Of these, 91 projects were from the focal topics of magnetism and superconductivity, materials sciences, crystallography and archaeometry. 61 projects were from the fields of soft condensed matter, biology and the life sciences.

WATCHING CATALYSTS AT WORK

A group of scientists at HZB observed **catalytic processes** at the atomic level using an innovative combination of methods. Their results should help in the development of new catalysts.

Developing materials with novel catalytic properties is one of the most important tasks in energy research. It is crucial to know exactly what is going on at the atomic scale in the dynamic processes involved in catalysis, such as the making and breaking of chemical bonds, or so-called ligand exchange reactions. Scientists from Helmholtz-Zentrum Berlin (HZB) and collaborators combined the spectroscopic method RIXS with *ab initio* theory to characterize these processes in detail for a metallic molecule complex of great interest to catalysis research: the iron carbonyl complex.



Elementary processes in the limelight: Donor and acceptor binding properties of the model catalyst $Fe(CO)_5$ in solution are studied by resonant inelastic X-ray scattering.

Studying chemical bonds directly

Iron carbonyl complexes are used in a vast number of chemical reactions and industrial processes, including light-induced water reduction and the catalytic removal of carbon monoxide from exhaust gases. Their catalytic action results from the rapid formation and subsequent breaking of chemical bonds between the metal centre and the carbonyl ligands. "It is essential for us to be able to determine the strength of orbital interactions in carbonyl complexes by observing the metal centres and the ligands directly," says Prof. Dr. Emad Flear Aziz, head of the HZB junior research group 'Structure and Dynamics of Functional Materials'. Until recently, direct observation during homogeneous catalysis in solution had been impossible. Now, with the development of the HZB junior group's new "LiXEdrom" experimental station for taking measurements in a microjet of liquid, it is possible to perform RIXS (resonant inelastic X-ray scattering) experiments on functional materials under in-situ conditions.
In collaboration with scientists from various universities, Aziz's team has now successfully studied both the metal and the ligands under the real application conditions in which this catalyst is used (in situ) using RIXS spectroscopy at HZB's electron storage ring BESSY II. They discovered a very strong orbital interaction between the metal and its ligands, which led to a weakening and elongation of the chemical bond during RIXS excitation.

Combining theory and research

The experimental results were supported by theoretical *ab initio* methods by the University of Rostock. "With this new combination of methods, we have gained fundamental insights into the electronic structure of iron carbonyl complexes under catalysis-relevant conditions," Aziz reports. "Our approach can help provide a better understanding of reaction dynamics and metal–ligand–solvent interactions on very short time scales. This leads to better control of catalytic properties – and holds great potential for the production of novel catalytically active materials."
The work was a collaboration with Prof. Dr. M. Bauer (Faculty of Chemistry, TU Kaiserslautern), Prof. Dr. J.-E. Rubensson (Dept. of Physics and Astronomy, Uppsala University) and Prof. Dr. O. Kühn (Institute of Physics, University of Rostock).

hs

Angewandte Chemie, International Edition, Vol. 52, Is. 37, pp. 9841-9844 (DOI: 10.1002/anie.201303310): Direct Observation of Molecular Orbital Mixing in a Solvated Organometallic Complex, E. Suljoti, R. Garcia-Diez, S. I. Bokarev, K. M. Lange, R. Schoch , B. Dierker, M. Dantz, K. Yamamoto, N. Engel, K. Atak, O. Kühn, M. Bauer, J.-E. Rubensson and E. F. Aziz

SEEING INTO THE HEARTS OF BATTERIES

Lithium-ion batteries lose capacity every time they are charged. A research group at HZB investigating the chemical processes in the **charging process** has discovered an effect that could explain this phenomenon.

In order to improve the lithium-ion batteries in electric vehicles, scientists at HZB studied the charging process at the atomic scale.

Lithium-ion batteries are the stars among the chemical energy stores. They are the first choice when it comes to powering smartphones and tablet computers, and even electric vehicle manufacturers swear by the long-lasting, robust lithium-ion–based cells. Yet, if they are to deliver the performance we have come to expect from our automobiles, these batteries still have a long way to mature – especially when it comes to energy density, which determines the weight of the battery and the range of the electric vehicle. "Crucial to this are microscopic processes taking place at the cell's electrodes upon charging and discharging," says Roland Steitz, chemist at the HZB Institute for Soft Matter and Functional Materials.

In principle, lithium reacts reversibly with other substances to form chemical compounds. In these processes, lithium atoms are embedded into the electrode material and then forced out again. "This happens very slowly, which is why it takes so long for a battery to charge," Steitz says. "The atomic processes gradually age the battery." But nobody had ever known what exactly happens at the interface between the electrodes and the electrolyte – the conductive substance that separates the two electrodes.

This is mostly due to the enormous difficulty of observing the atomic processes in situ, i.e. what actually happens inside an intact cell. Now, seemingly insurmountable hurdles have been overcome: together with Harald Schmidt, head of the Microkinetics workgroup at the Institute of Metallurgy of Clausthal University of Technology, and a team of scientists from several other German research institutes, Roland Steitz has demonstrated how to look deep into the heart of a battery: by neutron scattering on the lithium atoms.

Watching the charging process with neutrons

At HZB, the researchers trained their beam of neutrons on a battery electrode made of amorphous silicon – a promising candidate material for a new generation of especially high-capacity lithium-ion batteries. They applied a layer of this material onto a quartz substrate, which they enclosed in an airtight capsule. As a counter-electrode, they used metallic lithium. While applying an electric voltage to the battery, the researchers fired a beam of neutrons at the cell. Computer simulations helped interpret the neutron scatter patterns and discern the microscopic structures inside the cell.

"In this way, we were able to observe directly how lithium penetrated into the electrode and distributed itself throughout it," Steitz reports. "We also observed how the electrode expanded as the lithium was embedded – because the structure of the silicon changed." The researchers were surprised to discover that during the reverse process as the lithium ions left the amorphous silicon, a solid, lithium-rich layer formed a few nanometres thick on the surface of the electrode. "This could be one reason why lithium-ion batteries gradually and irreversibly lose capacity upon charging and discharging", the HZB researcher concludes.

He and his colleagues will be following up on this discovery in further experiments. Their aim is to help improve the properties of lithium-ion batteries – and push the door further open to a wide range of applications and a giant market. *rb*

Phys. Chem. Chem. Phys., 2013, 15, 7777 (DOI: 10.1039/c3cp44438d): Neutron reflectometry studies on the lithiation of amorphous silicon electrodes in lithium-ion batteries, B. Jerliu, L. Dörrer, E. Hüger, G. Borchardt, R. Steitz, U. Geckle, V. Oberst, M. Bruns, O. Schneider and H. Schmidt

SHEDDING LIGHT ON MAGNETOELECTRIC COUPLING

What if we used ferroelectric and magnetic properties interdependently in a single system? A research group from the Center for Nanointegration (CENIDE) at the University of Duisburg-Essen (UDE) has done just that in a **composite system**, which they studied at BESSY II.

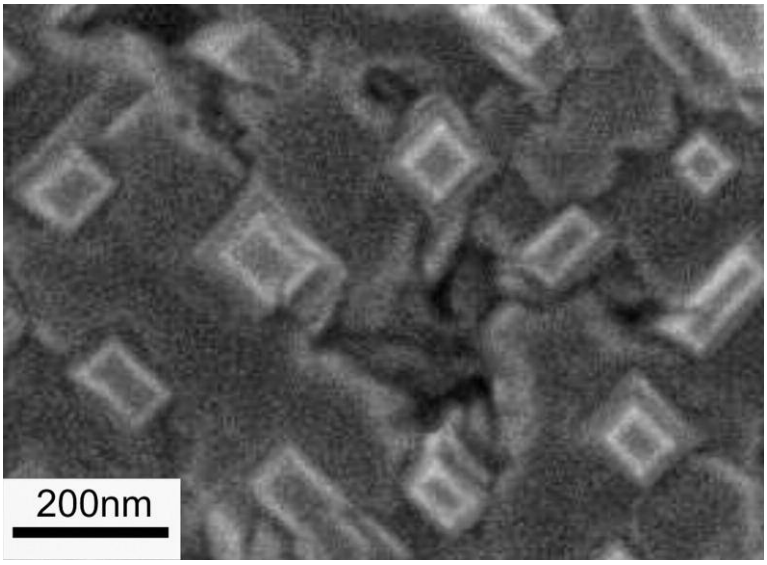
At the end of the 1950s, American physicist and later Nobel laureate Richard Feynman prophesized that all the knowledge in the world could one day be stored in a memory system no bigger than a grain of sand. While the first computers 70 years ago boasted only a few kilobytes of memory capacity and filled entire halls, these days we can store terabytes of information in the space of a lunchbox. Yet we have run up against the limits of our present technology – the existing system cannot be shrunk down any further or made any faster. That means we need new technologies for our increasingly complex demands.

Research for future storage media

The scientists of CENIDE are conducting research that could very well provide the basis for novel storage media. Experimental physicists Prof. Dr. Heiko Wende, Prof. Dr. Wolfgang Kleemann and Dr. Carolin Schmitz-Antoniak and their group are studying a system consisting of a layer of barium titanate into which teensy pillars of cobalt ferrite only a few nanometres long are embedded. The two components in this composite are very different: the pillars are ferrimagnetic, i.e. they align themselves to a magnetic field like tiny compass needles. They can also be deformed by a magnetic field. By contrast, the surrounding layer, or matrix, is ferroelectric and builds up an electric potential when mechanical pressure is applied. This is the piezoelectric effect as used in flintless lighters, for instance: when you press the button, a spring flicks a hammer onto the piezo crystal to produce a high electric voltage. This produces a spark at the nearby metal contacts, which ignites the lighter gas.

Precise compression of nanopillars

The scientists' aim is to use a magnetic field to deform the nanoscale pillars and thereby exert mechanical pressure on the matrix. This is referred to as "magnetoelectric coupling of a multiferroic composite system", a research field of great interest and of high application relevance worldwide. Magnetoelectric coupling is actually based on tiny movements of the atoms in the composite: when a magnetic field is applied along the long pillar axis, the pillars contract in that direction. Their circumference expands in the process to keep the volume constant, whereupon they press on the surrounding matrix on all sides. Under the resulting pressure, the matrix builds up an electric voltage.
If the magnetic field runs transversely across the pillars instead, then as they contract in the direction of the field they expand perpendicularly to it. That compresses the matrix only perpendicularly to the magnetic field, forming an asymmetrical electric polarisation distribution that has never been observed before in this system.
The system is especially interesting for digital data storage because the electric polarisation persists even when the magnetic field is switched off again. The researchers have



Scanning electron micrograph of the barium titanate layer in which the tiny pillars of cobalt ferrite measuring only a few nanometres are embedded.

The researchers used soft and hard X-rays for their experiments which are available at two different beamlines on BESSY II.

developed a strategy for compressing single nanopillars longitudinally or transversely using in a targeted manner pulsed currents as a way to write information bitwise.

Voltage instead of current

In principle, the process ought to work in reverse as well: the direction of magnetisation could be switched to write a bit using only electric potential, meaning without any current flow. The information would then be read out from the magnetic structure as usual. "Of course this is still a long way off," says workgroup head Wende, "but the magnetoelectric storage principle offers fundamental advantages." In the long term, it is highly energy efficient because it uses voltage only and there is no current flow. It also produces no heat, which would be greatly detrimental to the data integrity of the extremely densely packed storage elements. Furthermore, unlike various other high-tech concepts, magnetoelectric memories work at room temperature without expensive cooling, and store the data within them extremely stably. Nevertheless, many memory cells will be deleted and rewritten before compressed magnetic nanopillars are actually used to store our data.

Researching with soft and hard X-rays

The experiments were done at BESSY II using soft X-rays in the high-field chamber on beamline UE46-PGM1, exploiting the unique opportunity this chamber offers: here, you can rotate the applied magnetic field relative to the polarisation direction of the X-ray light used. By combining so-called circular dichroism with linear dichroism, the scientists gleaned information about the magnetism and electric polarization of the atoms involved. The experiments were performed in cooperation with Dr. Detlef Schmitz of the Institute for Complex Magnetic Materials.
Furthermore, in cooperation with Dr. Esther Dudzik and Dr. Ralf Feyerherm of the same HZB institute, they conducted experiments using hard X-rays on the MAGS beamline. The information they gathered on the crystalline structure confirmed the deformation of the matrix by the applied magnetic field, which partially remains even when the magnetic field is turned off.

ih

Nature Communications 4:2051, 2013 (doi: 10.1038/ncomms3051): Electric in-plane polarisation in multiferroic $CoFe_2O_4/BaTiO_3$ nanocomposite tuned by magnetic fields; C. Schmitz-Antoniak, D. Schmitz, P. Borisov, F. M. F. de Groot, S. Stienen, A. Warland, B. Krumme, R. Feyerherm, E. Dudzik, W. Kleemann and H. Wende

IN BRIEF

- In terms of the storage capacity and the speed of the storage process, the current technology of data storage is nudging its physical limits.
- Materials in which ferroelectric and ferromagnetic properties can be controlled independently of each other could open the way to further miniaturisation of memory systems.
- A CENIDE research team managed to control the pillars of only a few nanometres in size within a composite material which they were studying at BESSY II.
- Further research, however, is still necessary before the magnetoelectric storage principle can be used in practical applications.

ANTIQUE COINS UNDER NEUTRON FIRE

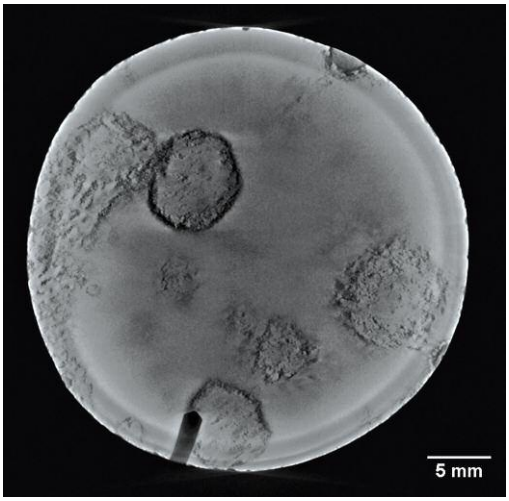
Scientists working with Gerald Eisenblätter have discovered **defects in the cores of antique Roman coins** using computer tomography. These point to degradation processes, which must be stopped.

At the beginning of the 19th century, the pioneers of archaeometry, or the science of archaeology, must surely have wished they could peer inside antique coins without destroying them. Gerald Eisenblätter of the University of Leipzig is testing out this very possibility. He is using X-ray computer tomography to analyse ancient coins for their metal composition, the density distribution within and accordingly their state of preservation, the key point being that the X-rayed objects remain undamaged.
X-ray computer tomography is used very often in medicine and in the materials sciences these days – particularly for the non-destructive testing of structural elements. Its use in archaeometry, on the other hand, is still very rare. Gerald Eisenblätter explains the imaging method: "When we shine X-rays through an object, the object absorbs some of them; the polychromatic X-rays are diminished." Given density differences inside the sample, a specific image emerges in the escaping rays, the materials scientist explains. If you capture many projections of the sample from different angles, then you get a high-precision, three-dimensional image that reveals additional information about the internal composition.

Second measuring technique as control

In this way, Gerald Eisenblätter and his team in the workgroup of Prof. Dr. Klöß dispelled all doubt as to the authenticity of the Roman copper pieces studied. They also revealed a weak point in an earlier appraisal: "We showed that the drilling from the first analysis was done in areas that were internally corroded." Which is not to say the scientists didn't encounter problems of their own: for instance, the appearance of disruptive effects called beam hardening artefacts. These are bright patches that show up in the X-ray image which can lead to false interpretations. "This effect doesn't exist for neutron tomography, because the measurement geometry is different," Eisenblätter explains. The researchers therefore found the solution to this problem at HZB in Berlin. Together with HZB scientists Alexandra Franz, Nikolay Kardjilov and Stefan Zander, they used the neutron computer tomograph CONRAD (V7) and the neutron powder diffractometer FIREPOD (E9) to reveal the missing information on the coins' internal composition. It turns out that the brass alloy had become completely unmixed in certain places, which now consist of copper alone. Under weathering processes, the zinc had separated out of the brass. This is what led to the misleading results of the first analysis. "It is a reminder to us that analyses made using invasive or exclusively surface-sensitive methods still have to be backed up by controls," Eisenblätter says.
The finding that will certainly interest historians and conservators is that about 20 percent of the 120 coins analysed so far possess internal defects, as Eisenblätter reports. In other words, one in every five coins has suffered degradation processes, which could still be ongoing. Now they are faced with the task of identifying the causes of this process, which could perhaps be special ions. Once identified, the degradation processes in historical coins might then be halted in a targeted manner.

ht



2D X-ray computer tomogram of the Tiberius sesterce taken from the collection in the Duke Anton Ulrich Museum in Braunschweig. Shown is the core of the coin with the drilled hole hailing from an earlier analysis (bottom left) as well as two points of zinc depletion (round surfaces).

Arbeitstitel – Forum für Leipziger Promovierende, Bd 5, Heft 1 (2013). S. 30–37, Ein Blick in das Innere antiker römischer Kupfermünzen. Eine Analyse mittels 3D-Röntgencomputertomographie, Gerald Eisenblätter

A LITTLE ALUMINIUM GOES A LONG WAY IN METHANOL PRODUCTION

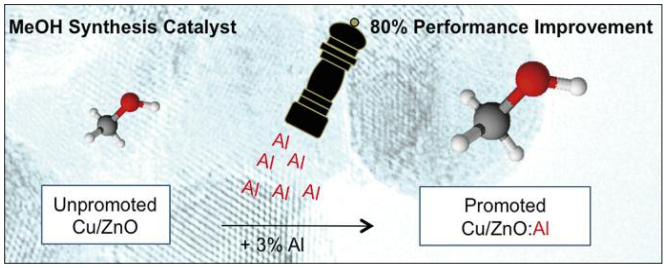
Methanol can be used as a **carrier for renewable energies**. Prof. Dr. Malte Behrens of the Fritz Haber Institute and colleagues are working on improving the catalysts used in methanol synthesis.

At certain times, wind turbines and solar cells deliver so much electricity that there are not enough consumers to make use of it all. Since only some of the excess electricity can be stored in batteries, the rest could be used to produce methanol. The chemical industry namely requires 50,000 tonnes of this alcohol each year for a host of its products. On top of that, methanol is being increasingly added to petrol. If this methanol is synthesized directly from hydrogen and carbon dioxide, then the alcohol will even burn carbon-neutrally, since it will only release the amount of carbon dioxide that was bound during its production. There is another advantage to this method: industry has long employed catalysts to produce methanol this way at relatively low cost. Until recently, however, no one has known exactly how these catalysts work. Malte Behrens of the Berlin Fritz Haber Institute of the Max Planck Society and colleagues have now changed that by experimenting with soft X-rays from the synchrotron source BESSY II at HZB.

Uneven distribution discovered

The catalyst production process uses a copper oxide/zinc oxide mixture from which hydrogen removes a certain amount of oxygen. Until recently, researchers had assumed the hydrogen reduces only the copper oxide, forming metallic copper. This copper would in turn activate the hydrogen so that it reacts easily with carbon dioxide. It was the job of the zinc oxide to prevent clumping of the copper and, with it, prevent a sudden drop in the catalyst's performance.

When Malte Behrens and colleagues replaced zinc oxide with the similar magnesium oxide, the catalyst no longer worked. The researchers therefore looked deeper into zinc oxide's exact role in the process. For this, they observed the catalysts at work using soft X-rays from BESSY II. The higher the energy of these beams, the deeper they penetrate into the material surface. They revealed surprising differences: The inside of the catalyst contained around 80 percent copper and 20 percent zinc, while its surface presented more zinc than copper.



Three percent aluminium increases methanol catalyst performance by as much as 80 percent.

Research on further improvements

Malte Behrens offers an explanation for this distribution: during production of the catalyst, the hydrogen also removes a small amount of oxygen from the zinc. This results in a mixture of zinc and zinc oxide, which slowly creeps to the surface. The zinc in this mixture apparently activates the carbon dioxide, making it convert more readily into methanol. The fact that adding a little aluminium greatly improves the performance of such a methanol catalyst supports this hypothesis. In the best catalysts, aluminium attaches mainly to the zinc oxide. Behrens suspects the aluminium increases the mobility of the zinc/zinc oxide mixture, which then migrates more easily to the surface of the catalyst. Behrens is currently researching on further improvements to catalysts for methanol synthesis – such as adding the metal zirconium, which Behrens believes could increase the mobility of the zinc/zinc oxide mixture even further.

rk

Angewandte Chemie, Vol. 125/Is. 25, p. 6664-6669 (DOI: 10.1002/ange.201301419): Die Rolle der Oxidkomponente für die Entwicklung von Kupfer-Komposit-Katalysatoren zur Synthese von Methanol, S. Zander, E.L. Kunkes, M.E. Schuster, J. Schumann, G. Weinberg, D. Teschner, N. Jacobsen, R. Schlögl and M. Behrens

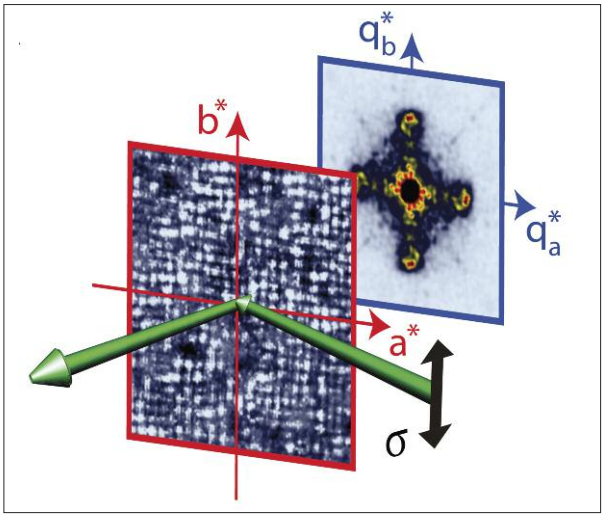
RIGID ORDER COMPETES WITH SUPERCONDUCTIVITY

The charge carriers in cuprate high-temperature superconductors can arrange themselves into **tiny "nanostripes"**. Guest researchers from Princeton and Vancouver working at BESSY II have shown how this supresses superconductivity.

Superconductors are materials that conduct electricity without any loss of energy. Before they exhibit this property, however, classic superconductors have to be cooled to almost absolute zero (minus 273 degrees Celsius). There are also "high-temperature" superconductors, but "high" is relative: they still only work at a freezing minus 200 degrees Celsius. While this cooling is difficult and expensive, superconductors have already paid off in many real-world applications such as magnetic resonance imaging (MRI) in medicine, for instance. In spite of all efforts, there are still no materials known to superconduct electricity at room temperature.
High-temperature (Tc) superconductors were discovered in 1986 and their discoverers received the Nobel Prize one year later. High-Tc superconductivity occurs in a class of materials known as the cuprates, which are complex compounds of copper and oxygen plus various other elements. Despite all the research that has been done over the years, there are crucial processes that are still not fully understood. The way charge carriers behave in these materials, for instance, depends on many subtle details and a whole host of mechanisms resist their transition to a superconductive state. Other material states compete, as it were, with the superconductive state.

Investigating nanostructures in the charge order

One of these competing states arises when the charge carriers arrange themselves into a regular, nanoscale stripe pattern. This arrangement immobilizes the charge carriers, thereby suppressing superconductivity. Back in 2012, guest researchers at BESSY II elucidated the importance of this mechanism and its connection with superconductivity in an important group of cuprates. Led by two research groups from Vancouver and Princeton, international teams have now detected this same charge order in other cuprates as well, identifying it as a fundamental property of this class of materials.
They did this using the XUV diffractometer developed by HZB and operated at the UE46_PGM1 beamline at BESSY II. Employing soft X-ray synchrotron radiation, they were able



Stripe pattern of charge carriers in $Bi_2Sr_2CaCu_2O_{8+x}$. The figure shows the structure with a period of about one nanometre (front) and the associated diffraction pattern (back) in the form of a so-called Fourier transformation.

to measure these elusive nanostructures in the charge order with high precision, making a significant contribution to our understanding of this phenomenon. The research involved the close collaboration of scientists from the department Quantum Phenomena in Novel Materials at HZB. "Identifying and understanding the mechanisms competing with superconductivity raises the hope of controlling and eventually deactivating them. This may be one step towards superconductivity at room temperature," explains Dr. Eugen Weschke, who supervised the experiments at BESSY II.

arö

Science, 2013 (doi: 10.1126/science.1243479): Ubiquitous Interplay between Charge Ordering and High-Temperature Superconductivity in Cuprates; E. H. da Silva Neto et al.

Science, 2013 (doi: 10.1126/science.1242996): Charge order driven by Fermi-arc instability in $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$; R. Comin et al.

MINUTE WATER CURRENTS UNDER THE NEUTRON MICROSCOPE

Researchers at HZB have made significant improvements to **neutron imaging techniques** to improve the study of processes occurring within fuel cells.

Inside fuel cells, hydrogen reacts in a controlled fashion with oxygen from the air. This produces electric current, which can run an electric motor. The product of the reaction is water. For applications in cars or in fuel-cell power plants, engineers prefer so-called PEM fuel cells. A thin film – called a polymer electrolyte membrane (PEM) – keeps hydrogen and oxygen separate from each other. Only protons, the nuclei of hydrogen atoms, can penetrate this membrane in a chemical reaction. The PEM must be kept constantly saturated with water to guarantee optimum proton conductivity. And yet, water that forms and collects on one side of the membrane can impair the cell's function by blocking the reactive gases.

The developers are working on preventing this disturbing effect as largely as possible by modelling and simulating the processes within the cell. This requires precise knowledge of the mechanism by which water penetrates into the membrane and distributes itself throughout. A group of scientists led by Nikolay Kardjilov, André Hilger and Ingo Manke of the Institute for Applied Materials Research of HZB has now shown – together with researching colleagues from the University of Tennessee in Knoxville (USA) – that slow neutrons are excellent for analysing this at high resolution. For their study, they used "cold" (low-energy) neutrons at HZB's instrument CONRAD (Cold Neutron Tomography and Radiography). The scientists fired these neutrons at a PEM while water-vapour–enriched nitrogen flowed across it.

Cold neutrons for precise measurements

"Neutrons are absorbed by the water molecules while they pass through the other materials largely unhindered," explains Ingo Manke, head of the tomography group at HZB. "From the changes in neutron density after they had penetrated the sample, we were able to calculate the quantity and spatial distribution of the water." This technique, known in physics as neutron imaging, is already recognized as an excellent method in this context. Yet, as technology advances, fuel cell developers are forever building more efficient and thinner membranes, which nowadays require extremely sensitive measurements to study. To conduct their cold neutron study, the researchers – together with engineers from US automotive group General Motors – developed a special air-tight moisture cell. This cell contained the PEM fastened between two aluminium plates. As they directed humidified nitrogen over the membrane through fine channels, the researchers simultaneously fired neutrons at it. The entire system was heated to 80 degrees Celsius, the typical operating temperature of a PEM fuel cell. In order to follow the changes in water distribution over time, the scientists took a sequence of many neutron images at about 30-second intervals – essentially making a movie of the water diffusion process. Each of these images had a spatial resolution of around 30 microns. That allowed the materials researchers to detect water quantities of a mere 10 nanograms inside the membrane. "Such high measuring sensitivity to the minutest quantities of water in the PEM is so far unique," Ingo Manke is pleased to report. "The results demonstrate the power of imaging with cold neutrons – and they are promising for future studies of PEM fuel cells featuring even thinner membranes." *rb*

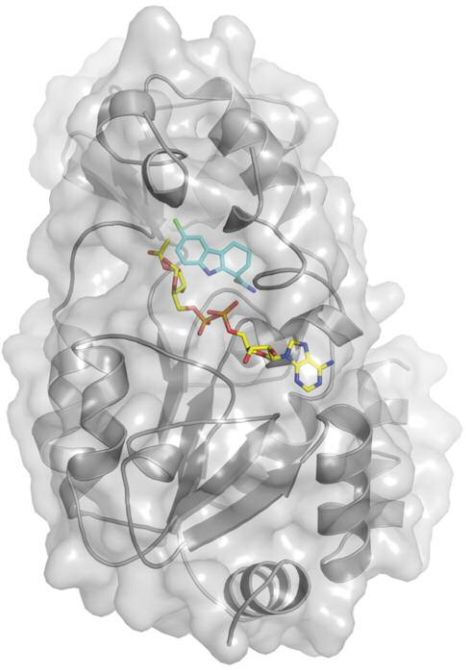
The CONRAD instrument at Lise-Meitner-Campus of HZB in Berlin-Wannsee.

Appl. Phys. Lett. 102, 234102, 2013 (doi: 10.1063/1.4811246): Detection of water with high sensitivity to study polymer electrolyte fuel cell membranes using cold neutrons at high spatial resolution; J. R. Bunn, D. Penumadu, R. Woracek, N. Kardjilov, A. Hilger, I. Manke and S. Williams

MEDICAL RESEARCH AT THE MX BEAMLINES

The MX beamlines at BESSY II are perfectly suited to analysing protein structures. The **1000th protein structure** determined from measurements in Berlin was released into the public domain in 2013. The insights gained from this type of research often point the way to better medical therapies.

Proteins play a crucial role in many processes within the body. In order to understand what tasks they fulfil and how they interact with other molecules, researchers need to know their exact three-dimensional structure. The way they are folded can be revealed using X-ray structural analysis of protein crystals. This requires extremely brilliant X-ray light and special measurement conditions, as have been available for over ten years at the MX beamlines at BESSY II. "Over the last few years, we have substantially improved the measuring station several times, as can be seen from the dramatically increased throughput," says Dr. Uwe Müller, who installed the MX beamlines at BESSY II and is in charge of the scientific use and maintenance of the instruments.



The inhibitor Ex-527 binds to the enzyme Sirt3 (light grey surface) as well as to acetylated ADP ribose, which is a direct product of Sirt3-mediated deacetylation. With ADP ribose now bound to the enzyme, the sirtuin's active site remains blocked, thereby preventing further deacetylation processes. On its first action, the sirtuin effectively sets itself a trap from which it cannot escape.

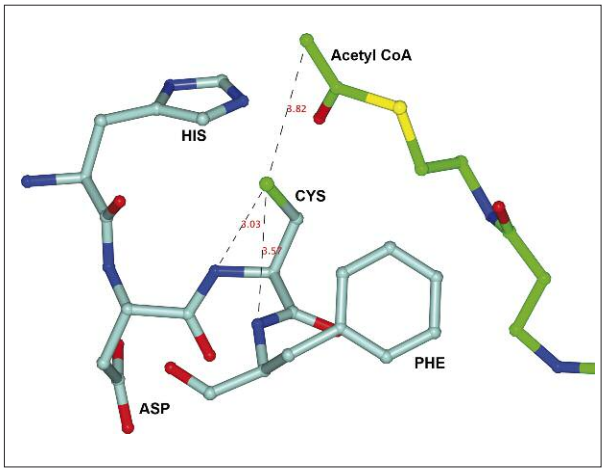
Researchers of Bayer Healthcare Pharmaceuticals Berlin had decoded the 500th protein structure as recently as 2010. "Only two years later, in May 2012, the Steegborn group took the measurements that have now led to publication of the 1000th structure in the summer of 2013," says HZB scientist Dr. Manfred Weiss, who manages the MX beamlines alongside Müller.

Medically exciting results

Analysis of the 1000th protein, which belongs to the class of sirtuins, is a special highlight that could be of major significance to medical research: sirtuins regulate metabolism, stress responses and aging processes in the body. Certain sirtuins – such as Sirt1 and Sirt3 – also play a role in the onset of cancer. Using drugs to inhibit their activity in a targeted manner is therefore an interesting approach for new cancer therapies. With their analysis, Prof. Dr. Clemens Steegborn at Bayreuth University and his group have explained how the activity of Sirt1 and Sirt3 can be suppressed by the molecule Ex-527.f "Our research results show that Ex-527 is an inhibitor with an unusual and simultaneously highly sirtuin-specific action," Steegborn explains. "If we are able to use what we have learned to specifically inhibit the activity of individual sirtuins, then this could be one approach to an effective therapy with only minimal side-effects," Steegborn reports optimistically. These results obtained from basic research are accordingly of great interest for medical research and for the development of active agents. In October 2013, the MX beamline scientists celebrated the 1000th publication with a symposium, at which Clemens Steegborn received an award.

Blocking the active site of thiolase

Further success was had by scientists of the University of Oulu, Finland, and of HZB: their research at the MX beamline has revealed new approaches for developing drugs against African sleeping sickness and other parasitic tropical diseases. Millions of people fall ill and thousands die from this disease every year. Drugs against the parasites are expensive and often have severe side-effects. No new, effective therapeutic agents have been developed for decades. The World Health Organization, WHO, therefore accords special importance to research into the development of suitable active agents.



Active site of the enzyme thiolase, which is essential for lipid metabolism in the parasites that cause African sleeping sickness. A main feature of the active site of trypanosomal thiolase is a specific loop deep within the protein molecule, the so-called HDCF loop (HIS-ASP-CYS-PHE), shown in light blue.

Scientists led by Prof. Rik Wierenga of the University of Oulu have prepared the ground for this by explaining the structure of the enzyme thiolase. Thiolase is essential to the parasites for lipid metabolism. “The key is knowing the geometry of the enzyme’s active site,” says Wierenga. “This is the place where lipids that play a central role in parasitic metabolism attach and where chemical reactions that convert lipids into other substances take place.” Knowing the structure and function of the active site allows one to develop substances that imitate lipids and attach firmly to the active site and thereby block it. The molecules involved are excellent starting points for developing new drugs.

The measurements of thiolase at BESSY yielded a highly detailed image of the enzyme’s active site: “The measurements of crystalline thiolase proteins we obtained at our MX beamline have helped to unravel the active site’s geometry,” says Dr. Manfred Weiss of HZB. One particular region of the protein, called the HDCF loop, turns out to be key. This structure, which lies deep within thiolase’s interior, was previously unknown. “Understanding the HDCF loop is the ideal starting point for developing new anti-parasitic drugs,” Rik Wierenga sums up.

hs/arö

PNAS 2013; July 8, 2013 (doi: 10.1073/pnas.1303628110): Ex-527 inhibits Sirtuins by exploiting their unique NAD+-dependent deacetylation mechanism; M. Gertz, F. Fischer, G. T. Tuyet Nguyen, M. Lakshminarasimhan, M. Schutkowski, M. Weyand and C. Steegborn

Biochem J., 455, 119-130 (doi: 10.1042/BJ20130669): Crystal structures of SCP2-thiolases of Trypanosomatidae, human pathogens causing widespread tropical diseases: the importance for catalysis of the cysteine of the unique HDCF loop; R. K. Harijan, T. R. Kiema, M. P. Karjalainen, N. Janardan, M. R. Murthy, M. S. Weiss, P. A. Michels and R. K. Wieringa

REVISIONS TO THE MX BEAMLINES

Since February 2013, the new detector PILATUS-6M on MX beamline BL 14.1 allows extremely precise insights into the complex folding of the building blocks of life. “For our users, the PILATUS detector is another giant leap forward. Given its size, its minimal noise and its speed, PILATUS-6M is the best there is at the moment when it comes to detectors for X-ray crystallography,” says Dr. Uwe Müller, head of the HZB workgroup Crystallography. The new machine was developed and manufactured by the Swiss company Dectris. HZB invested 1.2 million euros into this project.

Uwe Müller (left) and Thomas Frederking, Administrative Director of HZB, cut the ribbon for the new Pilatus 6M detector in February 2013.

The MX team working with Dr. Uwe Müller and Dr. Manfred Weiss is furthermore converting MX beamline BL 14.2 into a dedicated fragment screening beamline. In the joint research project “Frag2Xtal” funded with 640,000 euros by the Federal Ministry for Education and Research, MX beamline BL 14.2 is being upgraded to a high degree of automation. This will considerably reduce the effort of recording and evaluating hundreds to thousands of crystallographic datasets, and will thereby make certain experiments, for example in drug development, possible for the first time.

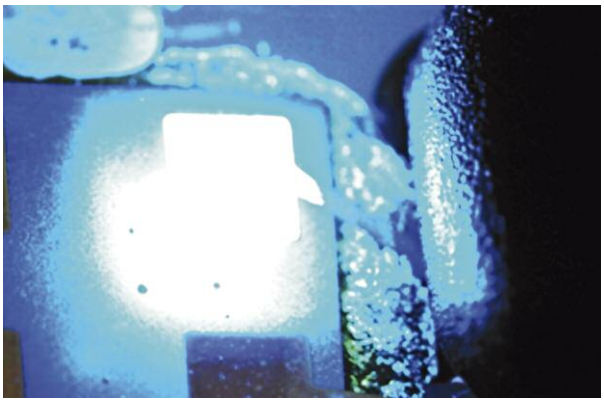
PRINTED DISPLAY SCREENS

Organic light-emitting diode (OLED) screens consume far less energy than conventional screens. A group led by Prof. Dr. Emil List-Kratochvil of the Graz University of Technology has researched how to manufacture them at lower cost.

A quarter of the electricity generated on earth flows through light bulbs and display screens. In the name of lowering this consumption, there is a popular movement towards light-emitting diodes (LEDs). While solar cells produce electricity from light, LEDs turn this reaction around and produce light from electricity. For much of their history, LEDs have been made with semiconductor materials such as gallium compounds. Nowadays, however, we also have OLEDs, which use organic molecules to produce light from electricity. "An OLED display not only consumes half the energy of a conventional liquid crystal display, it is also significantly brighter and has a higher contrast," explains Emil List-Kratochvil, who researched these organic light-emitting diodes at the Graz University of Technology and at the NanoTechCenter Weiz in Styria.
The first OLED products are already in circulation with production at around 20 million displays per month. So far, these OLEDs have been manufactured by vapour deposition in a vacuum and are therefore relatively expensive. Organic LEDs could be produced significantly cheaper if the constituent molecules could be dissolved into a liquid and printed like ink. Emil List-Kratochvil and his co-workers are investigating this possibility together with colleagues such as Prof. Dr. Klaus Müllen of the Max Planck Institute of Polymer Research in Mainz and Prof. Dr. Norbert Koch of Helmholtz Zentrum Berlin.

Printing is cheaper than vapour depositing

As is so often the case, the devil is in the details with such a technology. OLEDs are constructed as two ultra-thin layers. The first layer can be printed on with relative ease. However, because the component molecules dissolve in similar liquids, printing the second layer is problematic because the second application of ink immediately begins to dissolve the first printed layer beneath it. To prevent this decomposition, Emil List-Kratochvil and colleagues have introduced an intermediate step: they heat the first layer to 200 degrees Celsius in an argon atmosphere – protecting it against the aggressive oxygen in normal air – for one hour. This causes the molecules in this layer to crosslink and no longer dissolve when the second layer is printed on. The researchers can achieve the same effect if they modify the molecules of one layer to dissolve in other liquids that have not been used for these purposes so far, such as alcohol.
If the researchers now apply electricity to this printed OLED, electrons flow from one layer to the other, while so-called holes flow in the opposite direction from the second layer to the first. To ensure the negatively charged electrons and positively charged holes will not simply flow through the two layers without producing light, each layer is made of a different material. The transition between the two layers then forms an energy barrier that impedes both the electrons and the holes. This gives them time to unite and, in the process, rapidly emit a photon.
To obtain as much light from electricity as possible, not only must the individual layers rest precisely on top of each other, but the energy barrier between the two must also be optimally adjusted. This is exactly what Emil List-Kratochvil and his researchers are measuring with photons from the synchrotron source BESSY II. *rk*



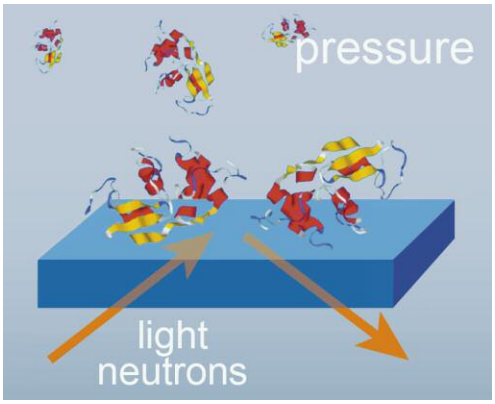
Organic light-emitting diodes not only illuminate more efficiently than LEDs, they can be manufactured by printing as well.

Advanced Functional Materials; Vol. 23/Is. 39, p. 4897–4905; (DOI: 10.1002/adfm.201300360): Bright Blue Solution Processed Triple-Layer Polymer Light-Emitting Diodes Realized by Thermal Layer Stabilization and Orthogonal Solvents; R. Trattnig, L. Pevzner, M. Jäger, R. Schlesinger, M.V. Nardi, G. Ligorio, C. Christodoulou, N. Koch, M. Baumgarten, K. Müllen and E. J. W. List

ENERGY BARRIERS IN THE NEUTRON BEAM

The **unfolding of proteins** leads to problems in a wide variety of applications. Scientists working with Dr. Roland Steitz are therefore researching to understand the process in greater depth.

Anyone who has fried eggs in a cast-iron pan knows the almost inevitable problem: the egg bakes firmly onto the pan and can only be removed again with a good deal of effort. This happens when proteins from the egg unfold in the heat, which biochemists refer to as denaturing. A similar situation can arise when surgeons insert stents to keep patients' coronary blood vessels open. Proteins from the blood adhere to the mesh of metal or plastic. In some circumstances this can pose a risk of vascular occlusion, which the stent is actually intended to prevent. Because proteins tend to adsorb to surfaces in many other contexts, physical chemists like Roland Steitz of HZB and Claus Czeslik of TU Dortmund have good reason to spend years studying the processes involved.
"First, the proteins need energy to unfold," Roland Steitz explains. In their natural state, the long protein chains



It is possible to measure the behaviour of proteins (red) marked with fluorescent dye (yellow) on surfaces (blue) particularly well and non-disruptively using high pressures of up to 2,500 bar.

namely self-assemble into compact balls. The heat in a pan delivers more than enough energy to turn these back into a chain that can stick especially well to the cast-iron surface. In fact, the electrostatic attraction of a material is usually sufficient to unfold a protein far enough for it to mould itself to that surface.
So-called "soft" proteins only need to unfold a little way before they will adsorb, and require relatively little energy to do so. "Hard" proteins, on the other hand, need to undergo much greater deformation. "A much higher energy barrier has to be overcome for these," says Roland Steitz. The protein need not necessarily be heated to achieve this; even increased pressure unfolds proteins to a certain degree. The food industry exploits this phenomenon when pasteurizing milk – where it is normally heated quickly to 60 or 70 degrees to make the proteins of dangerous germs unfold far enough to kill the germs. The same can be achieved with high pressure – a method that better conserves the healthy milk proteins.

How high is the energy barrier?

Using classic methods, physical chemists can only measure the energy barrier in a roundabout way. Claus Czeslik and his colleagues, for example, marked one of 500 proteins with a fluorescent dye. The brighter the protein's surface glowed, the more dye had become adsorbed. Just as the hobby chef can gauge temperature from the colour of eggs in a pan, researchers can determine the energy barrier to overcome for triggering partial protein unfolding from the brightness of a fluorescent dye.
Using the neutrons from BER II, however, the researchers can directly measure how many layers of a protein, in this case lysozyme, rest on a surface and how much of the protein each layer comprises. That way, they can directly correlate the measured energy barrier with changes in the adsorbed proteins. This gives stent manufacturers, for instance, information from which to develop protein-repellent coatings. At the same time, the researchers learned they can measure the behaviour of proteins on surfaces especially well and non-disruptively under high pressure. Provided they have sturdy enough measuring chambers.

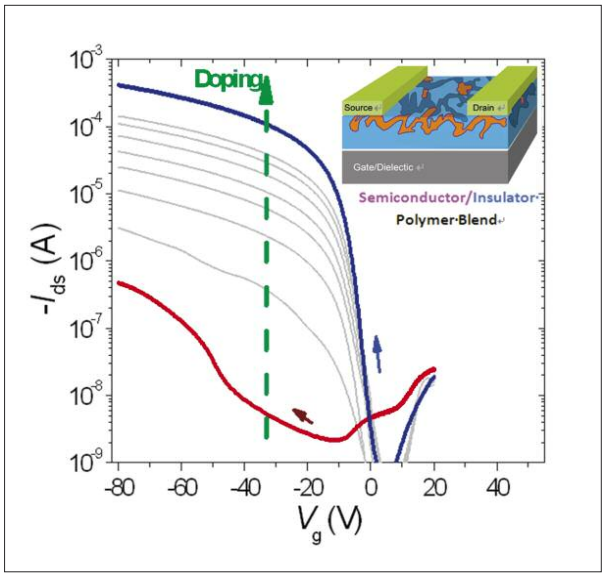
rk

ACS, Langmuir, 2013, 29 (25), pp 8025–8030 (DOI: 10.1021/la401296f): Pressure-Induced Protein Adsorption at Aqueous–Solid Interfaces; J. Koo, M. Erlkamp, S. Grobelny, R. Steitz and C. Czeslik

THE RIGHT DOPING MAKES ALL THE DIFFERENCE

Scientists working with Prof. Norbert Koch have figured out why moderate doping makes **polymer-based field effect transistors** work better. This could lead to improvements in actively controlled displays.

In organic electronics, blends containing semiconducting macromolecules embedded into an insulating polymer matrix have proven especially suitable for making transistors. Exactly why this is so, however, had long been unknown. Now, scientists from several research institutes have elucidated the complex morphology of these blends and thereby explained their electronic properties.
Organic semiconducting materials based on conjugated polymers currently achieve charge carrier mobilities comparable to or even superior to those of amorphous silicon.



The curve shows how, with increased doping in the semiconductor layer, the transistor ratio improves radically. The researchers ascribe this to the formation of conductive percolation pathways that facilitate the transport of charges along the transistor channel.

An especially interesting field of application for these materials is thin-film transistors, as used for backplanes in actively controlled displays, for instance. Semiconducting polymers, however, are not transparent; they are strongly coloured. Furthermore, these materials are doped with atmospheric oxygen, which leads to poor on/off ratios of the transistors. A number of years ago, it was shown that adding small quantities of semiconducting macromolecules to an insulating polymer matrix, say of polystyrene and polymethyl methacrylate (PMMA), allows the fabrication of transistors with excellent electric properties and with excellent stability in air. Yet, the extraordinary behaviour of this polymer blend has never been properly understood.

Doping creates conductive paths for charge transport

Scientists from the University of Potsdam and Humboldt-Universität zu Berlin, in collaboration with groups at Helmholtz-Zentrum Berlin für Materialien und Energie, the Max Planck Institute for Polymer Research in Mainz and Stanford University, were able to explain the structural and electric properties of these blends.
It turns out that in these blends, doping the semiconducting components leads to a drastic improvement in the transistor ratio. This is not observed in layers of purely conjugated polymers. The reason behind this is the complex morphology of the layers: Tiny grains of the semiconducting polymer are distributed inhomogeneously throughout the layer volume. In this complex structure, doping causes conductive percolation pathways to form, facilitating the transport of charges along the transistor channel. Furthermore, it takes only the depletion of a few semiconductor domains to turn the transistor completely off. By optimizing the blend, nigh-transparent organic field-effect transistors can be produced with mobilities of up to 0.3 cm2/Vs and very high on/off ratios.

arö

Nature Communications, Vol. 4, 1588, (doi: 10.1038/ncomms2587): Moderate doping leads to high performance of semiconductor/insulator polymer blend transistors; G. Lu, J. Blakesley, S. Himmelberger, P. Pingel, J. Frisch, I. Lieberwirth, I. Salzmann, M. Oehzelt, R. Di Pietro, A. Salleo, N. Koch and D. Neher

TRACKING DOWN DESTRUCTIVE RADICALS

There is much hope placed in **lithium-air batteries** for use in electromobility, yet they lose capacity every time they are charged. A research group working with Dr. Lada Yashina at HZB has discovered the causes for this flaw.

The future of mobility belongs to the electric motor, which will supersede fossil-fuelled internal combustion engines. Yet, electric vehicles have one weakness: their battery. The lithium-ion batteries used so far have too low an energy density, limiting the EV's range to 100 to 200 kilometres. Lithium-air batteries could make a hefty improvement, their energy density being around ten times greater. Yet, these batteries suffer from a flaw of their own: their capacity drops significantly with every charge process, meaning they become largely exhausted after only a few charge/discharge cycles. The cells contain a lithium electrode and an electrode made of a carbon material such as graphite or graphene. These materials have outstandingly high electric conductivity and a large specific surface area. On this surface, lithium ions react with atmospheric oxygen to produce lithium peroxide. "However, an insulating layer of carbonate forms at the same time," says Lada Yashina of the Chemical Institute of Moscow State University. This carbonate layer is the culprit behind the deteriorating battery capacity.
Yashina studied this disruptive process because it was previously unclear as to what chemical reactions were taking place inside the cell. Together with an international group of scientists, she managed to solve the puzzle – by performing experiments on the X-ray photoelectron spectrometer (XPS) of HZB. "The measurements were performed in the scope of a decade-long close collaboration between the two research institutes in Moscow and Berlin," the chemist reports. "The conditions for this are almost unique at HZB – since there are only few suitable spectrometers in the world."

A deeper look inside the battery

In order to characterize the chemical and electrochemical processes happening at the electrode, the researchers working with Lada Yashina and her Moscow colleague Daniil Itkis repeatedly charged and discharged a lithium-air cell while simultaneously measuring the photoelectron spectral curves. For the first time, they were able to follow the changes on the surface of the carbon in detail. The result presents a new picture of the deepest part of the battery:

Automobile manufacturers are still using lithium-ion batteries in electric vehicles such as this Nissan Leaf, but research is going full steam ahead in pursuit of better alternatives - not least through experiments at HZB.

During the charging process, highly reactive superoxide radicals form very briefly on the electrode and then combine with the carbon to form new chemical substances – including the disruptive carbonate. "It seems that defects in the carbon material that are associated with so-called functional groups play a crucial role in this," says Daniil Itkis. They present a favourable target surface for destructive superoxide attacks. The researchers confirmed this by experimenting with different carbon variants: Relatively defect-free graphite degraded significantly slower upon discharging than did graphene-oxide featuring substantially more defects.
"This inspires hope that lithium-air batteries can be optimised enough to be suitable for practical application in the future," Lada Yashina resumes. Yet, it would be essential to make them out of almost perfectly flawless materials, or to protect the carbon against the aggressive superoxides during discharging. The research group will be conducting further experiments to find out how this can be achieved. *rb*

Nano Letters 2013, 13, 4697–4701, (doi: 10.1021/nl4021649): Reactivity of Carbon in Lithium–Oxygen Battery Positive Electrodes; D. M. Itkis, D. A. Semenenko, E. Y. Kataev, A. I. Belova, V. S. Neudachina, A. P. Sirotina, M. Hävecker, D. Teschner, A. Knop-Gericke, P. Dudin, A. Barinov, E. A. Goodilin, Y. Shao-Horn, and Lada V. Yashina

DOMAIN WALLS AS INFORMATION STORES

At HZB, a research group from the Johannes-Gutenberg-University in Mainz has captured the **motion of magnetic domains** in minute nanowires for the first time. Their findings could push the door open to new applications.

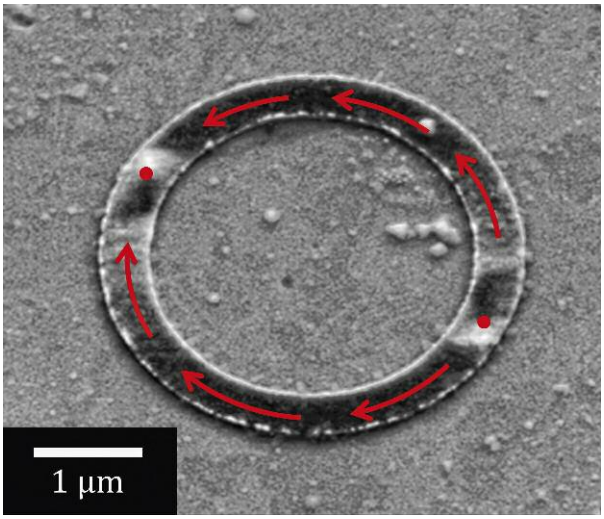
Ferromagnetic materials tend to form domains of uniform magnetisation within them. Where they border on each other, these domains form walls that can move and can even be manipulated in a targeted manner. The workgroup of Prof. Dr. Mathias Kläui at Johannes Gutenberg University Mainz has studied a class of domain walls that form as tiny magnetic rings of about four micrometres in diameter. These rings were made of permalloy, an easily magnetised ferromagnetic nickel-iron alloy.

Theoretical effects proven by experiment

The Mainz physicists collaborated closely with the groups of Prof. Dr. Gisela Schütz at the MPI for Intelligent Systems in Stuttgart and Prof. Dr. Stefan Eisebitt, who heads the joint research group "Functional Nanomaterials" of HZB and TU Berlin. With their measurements at the synchrotron sources BESSY II at HZB and the Advanced Light Source in Berkeley, USA, they were able to directly observe the motion of the domain walls under special X-ray microscopes. On the X-ray microscope MAXYMUS operated by the department of Prof. Schütz, for instance, they were able to record the processes in sequences of images. In doing so, they experimentally detected theoretically predicted effects and even detected new properties that promise interesting applications in information technology, as information stores or position sensors, for example.
Using rotating magnetic fields produced by pulsed currents, the researchers were also able to rotate the domain walls in the ring in a targeted manner. "The faster we rotate the domain wall, the easier it is to control it," says Dr. André Bisig from the group of Kläui, first author of the study. As they did so, they even observed a new effect: the speed of the domain walls fluctuates in this rotating motion, since the internal magnetic structure of the domain walls changes periodically.

Faster motion reduces the influence of defects

Another observation related to the effects of irregularities or defects in the nanowires. These effects only become noticeable when the domain walls move slowly. The faster a domain wall is rotated, the less of a role defects in the material play. "These results expand our understanding of the dynamic behaviour of magnetic domain structures," explains Stefan Eisebitt. "They also illustrate how important it is to be able to watch functional nanostructures 'at work' using modern X-ray microscopes, in order to derive new applications from the findings as well."



Scanning electron micrograph of a ferromagnetic ring that exhibits magnetisation (black & white contrast) along the ring and forms two domain walls.

Markus Weigand, head scientist at the MPI MAXYMU end station, further states: "Our scanning X-ray microscope at BESSY II is currently the world's most powerful instrument for direct time-resolved imaging of magnetization dynamics. The processes can be depicted in slow motion, slowed down by a factor of 'ten billion'."

arö

Nature Communications, Vol. 4, 2013, (DOI: 10.1038/ncomms3328): Correlation between spin structure oscillations and domain wall velocities; A. Bisig, M. Stärk, M.-A. Mawass, C. Moutafis, J. Rhensius, J. Heidler, F. Büttner, M. Noske, M. Weigand, S. Eisebitt, T. Tyliszczak, B. Van Waeyenberge, H. Stoll, G. Schütz and M. Kläui

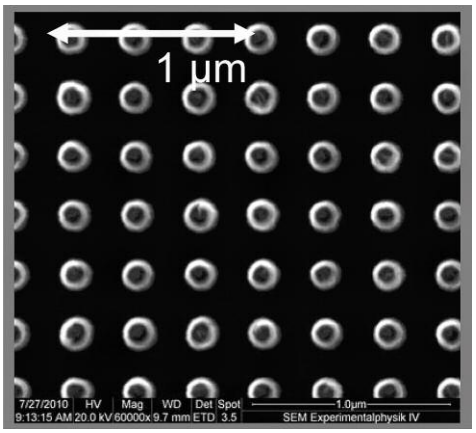
CHAINS, NOT ZIGZAGS

By performing measurements at BESSY II, physicists of Ruhr-Universität Bochum (RUB) have discovered how tiny islands of magnetic materials arrange themselves when sorted into a **regular lattice**.

Many atoms behave like a needle of a compass, i.e. they feature a north and a south pole like a tiny magnetic dipole. When crammed together into a crystal, one could expect all the dipoles to line up, making the material magnetic. But that is not the case. A material only becomes magnetic when special quantum mechanical forces are at work. In most cases, the forces between the atomic dipoles are much too weak to influence one another. Also, thermal energy jiggles the atoms about so much that, even at low temperatures, they point every which way in complete disorder. "Nevertheless, we are left with the fundamental question of how magnetic dipoles would arrange themselves if the force between them were strong enough," says Prof. Dr. Hartmut Zabel of the professorship for experimental physics/solid-state physics at RUB. "Understanding the driving interactions is of great technological interest for future hard disks, which will consist of tiny magnetic islands."
In search of answers, the researchers used lithographic methods to cut circular islands a mere 150 nanometres in diameter out of a thin magnetic layer. They ordered these islands into a regular square lattice. Each island contained about a million atomic dipoles. The forces between two islands were therefore a factor of one million stronger than those between two individual atoms. Leaving these dipoles to their own devices, one can then observe at low temperatures the alignment resulting exclusively from the interaction between the dipoles. They assume the most energetically favourable pattern – the so-called ground state. The islands in this system serve as a model for the behaviour of atomic dipoles.

Observing magnetic dipole islands

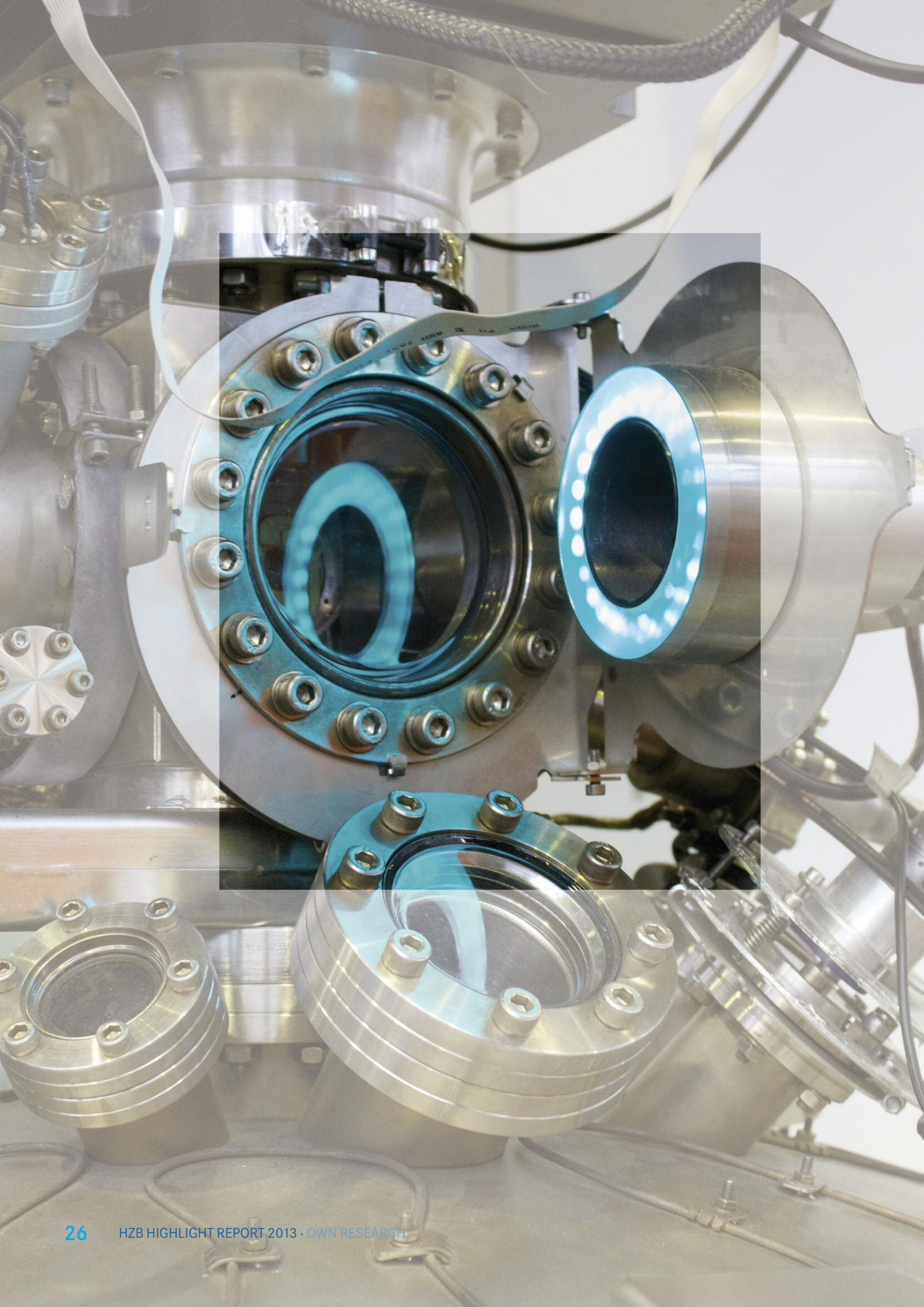
BESSY II is home to a special microscope: the photon emission electron microscope with which the RUB physicists revealed the alignment of the magnetic dipole islands. Using circular-polarized synchrotron light (X-rays), the device excites specific electrons. These reveal the alignments of the dipoles in the islands. The experiments were performed at low temperatures to ensure thermal motion did not disrupt the dipole alignments.



Scanning electron micrograph of a regularly arranged square lattice made up of magnetic islands. The researchers revealed the islands by means of electron beam lithography.

The magnetic dipoles formed chains where the north pole of one island would point to the south pole of the next island. "This result was surprising," Zabel says. In the lattice, each dipole island has four neighbours they could align to; there was no way to predict in advance where the north pole would ultimately point. "One would in fact expect a kind of zigzag arrangement," the physicist from Bochum says. From the chain pattern observed in the experiment, the researchers showed that higher-order interactions determine how the magnetization orients itself. There are not only dipolar interactions but also quadrupolar and octopolar interactions at play. That means a magnetic island exerts forces on four or eight neighbours at the same time. Future hard drives will consist of these tiny magnetic islands, where each magnetic island will form a storage unit that can represent the bit states "0" and "1" – coded by the alignment of the dipole. For a working computer, one needs an arrangement in which the dipole islands exert the least effect on one another, and can thereby assume the "0" and "1" states independently of one another. A precise understanding of the driving interactions between magnetic islands is therefore crucial for the technical application of this system. *hs*

Physical Review Letters, 2013 (doi: 10.1103/PhysRevLett.110.177209):
Magnetic Dipole and Higher Pole Interaction on a Square Lattice;
M. Ewerlin, D. Demirbas, F. Brüssing, O. Petracic, A.A. Ünal, S. Valencia, F. Kronast and H. Zabel



HIGHLIGHTS FROM OUR OWN RESEARCH

1,174 employees were employed at Helmholtz-Zentrum Berlin für Materialien und Energie in 2013, including trainees. 22 new training contracts were concluded; on 31.12.2013 there were a total of 57 young adults working in 11 trained professions at HZB. 323 women were employed at HZB, equating to around 27.5 percent of all employees.

487 ISI-cited papers were published by scientists at HZB in 2013. On top of these were 93 lectured publications, including the number of books and book contributions mentioned separately in the programmes. In total, 215 papers were from the field of renewable energies and 265 papers from photon, neutron and ion (PNI) research.

124 postgraduate students were supervised by HZB in 2013. In total, 28 doctoral theses, 6 diploma theses, 29 master theses, 23 bachelor theses and 2 student research papers were concluded. 59 postgrads worked in the field of renewable energies for their thesis and 65 in the field of PNI.

80 joint ventures with companies were entered into by HZB in 2013. The total number of ongoing joint ventures with industry at the end of 2013 was 181 – of these, 79 in the field of renewable energies and 88 in the field of PNI.

1**4 patents** were awarded by the German Patent and Trade Mark Office in 2013, of which 5 were in the field of renewable energies and 9 in the field of PNI. At the end of 2013, HZB's patent portfolio encompassed 345 national and international property rights, of which 235 were granted patents. 29 property rights were objects of ongoing licence agreements.

STRESSES IN GLASS

The transition from liquid to solid state creates internal stresses inside materials. Working in a research group, **Miriam Siebenbürger** has developed a model system for telling the two states apart with crystal clarity.

Many solid materials are produced by allowing a molten mass to solidify. Depending on how quickly it cools, internal stresses will almost always build up inside. A rather sensational example of this is Prince Rupert's Drops, also known as Dutch tears: the bulbous end of these glass drops can withstand a blow from a hammer without breaking, while even the slightest pressure on the thin end will cause the entire drop to disintegrate explosively. The properties of safety glass and gorilla glass are also governed by internal prestressing. Yet, so far, very little has been known about the specific properties that distinguish a glass state from a ductile, molten state. Using a surprisingly simple model, a cooperative of several research groups from Germany and Crete has now explained what distinguishes glass from molten mass.
One important contribution came from HZB: chemist Dr. Miriam Siebenbürger of the HZB Institute of Soft Matter and Functional Materials has developed an elegant model system consisting of plastic particles in aqueous saline solution, i.e. a colloid suspension. Because the particles are extremely small, around 150 nanometres in diameter, they stay floating in the solution without sedimenting out. These nanoparticles possess a thermosensitive "shell" whose thickness can be modified by heat, thus they can be made to continuously grow or shrink. The chemist can thereby control her samples to transition from a densely packed "glass" into a less dense, liquid state – melting it as it were. In a series of rheological experiments, Miriam Siebenbürger determined how quickly internal stresses could diminish in her samples at various packing densities.


Photo: HZB

Chemist Dr. Miriam Siebenbürger has developed a method for clearly distinguishing glass from liquid.

Experiment and theory agree

To do so, she clamped the samples between two plates which could be twisted in opposite directions in order to create shear forces in the sample. As soon as the material reached a stationary state of shear stress at constant shear speed, the plates were actively stopped. Next, the force required to hold the plates in the zero position was measured. This force is a gauge of the internal stresses. The crucial difference between the liquid and glass state became quite clear: while the stresses completely dissipated in the liquids, some of the stresses were permanently retained in the glass state.
These results match the theoretical model made by physicists from the University of Konstanz, who calculated the behaviour of hard spheres at various packing densities. But that is not all: measurements of the internal stresses and dynamics of larger particles (in the µm range) done by researchers in Crete and Düsseldorf and the molecular dynamic simulations of hard spheres by researchers in Cologne and Mainz exhibit the very same behaviour. The scientists are therefore confident their results can be applied broadly to all glasses formed by high packing density such as metallic glasses, as are being developed for high-tech applications. The work was published in the renowned Physical Review Letters, where it received the status "Selected for a Focus in Physics" and "Editor's Suggestion".

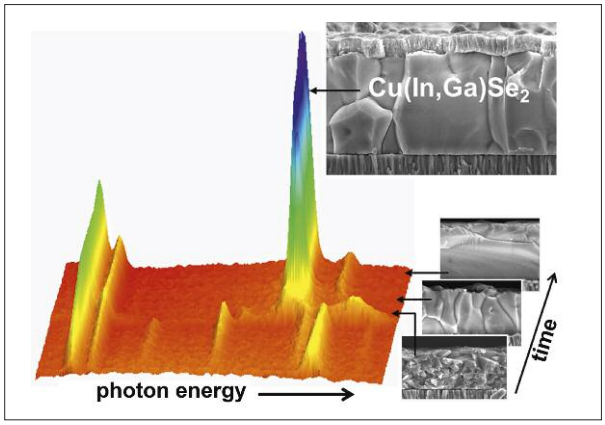
arö

Phys. Rev. Lett. 110, 215701 (2013), (DOI: 10.1103/PhysRevLett.110.215701): Residual Stresses in Glasses; M. Ballauff, J. M. Brader, S. U. Egelhaaf, M. Fuchs, J. Horbach, N. Koumakis, M. Krüger, M. Laurati, K. J. Mutch, G. Petekidis, M. Siebenbürger, Th. Voigtmann, and J. Zausch

WATCHING SOLAR CELLS AS THEY GROW

Scientists working with Dr. Roland Mainz and Dr. Christian Kaufmann at HZB are the first to successfully observe the **growth of high-efficiency chalcopyrite thin-film solar cells** in real time.

Chalcopyrite thin-film cells made of copper-indium-gallium-selenide (CIGS) already achieve efficiencies above 20 percent. So far, the most successful process for producing such extremely thin, polycrystalline layers is “co-evaporation”. This is where two different elements are vapour-deposited at the same time: indium (or gallium) and selenium in the first step, copper and selenium in the second step, and again indium (or gallium) and selenium in the third step. This builds up a covering of crystals with very few defects. “Until recently, however, we never knew exactly what happens during this co-evaporation,” says Dr. Roland Mainz of the Institute of Technology of HZB. The physicist and his colleagues worked for three long years to find a way to investigate this process in real time using local experimental equipment.



Growth of the layers can be analysed using in-situ X-ray scattering and fluorescence signals.

Novel experimental chamber with vacuum and heating elements

Their solution was to build a novel experimental chamber in which to study the formation of the polycrystalline chalcopyrite layer during co-evaporation using the synchrotron light from BESSY II. Alongside feed lines for the vaporized elements, the vacuum chamber contains heating and cooling equipment for controlling the vapour deposition process. Using this they were able, as a world first, to observe the growth of the polycrystalline layers using “in-situ” X-ray diffraction and fluorescence analysis in real time during the co-evaporation. “We now see how the crystalline phases convert from one to another during the various vapour deposition stages and how defects arise in the process. But we can also detect when these defects disappear again.”

This happens during the second step, when copper and selenium are vapour-deposited. Excess copper depositing as copper selenide on the surface helps smooth out the defects. “This was already known from earlier experiments, but we have now shown from the fluorescence signals and numerical model calculations that the copper selenide penetrates into the copper-indium-selenide (CIS) layer,” Mainz explains. This is where they observed significant differences: While copper easily penetrates into the CIS layer, it simply stays put on the surface of the otherwise highly similar compound copper-gallium-selenide (CGS). This could be one reason why pure CGS has failed to yield high solar cell efficiencies so far.

Processes can be accelerated partially

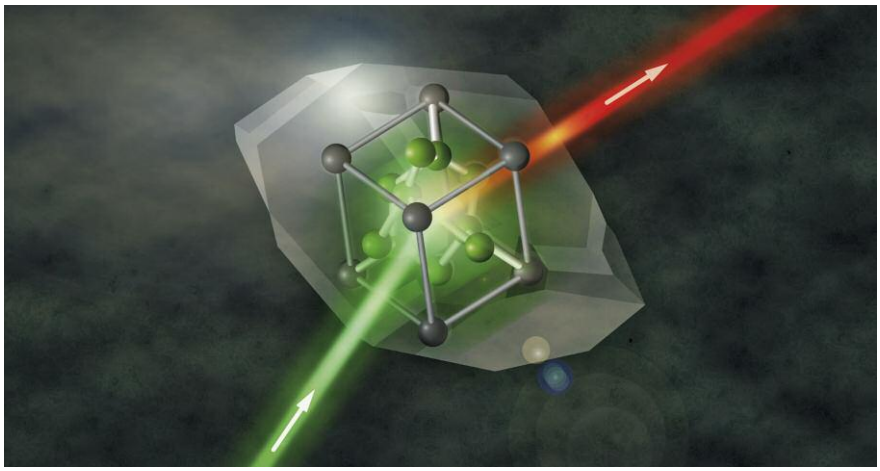
“Now we know where to start in order to optimise the process, namely at the transition into the copper-rich phase. The practice so far has been to run the process very slowly in all phases, to give defects the chance to fix themselves. Our results suggest that certain process phases can be accelerated and that the process only needs to run slowly wherever defects have to be optimally fixed,” Mainz explains. *arö*

Advanced Energy Materials, Vol. 3, Issue 10, pp. 1381-1387, Oct. 2013 (DOI: 10.1002/aenm.201300339): Formation of $CuInSe_2$ and $CuGaSe_2$ Thin-Films Deposited by Three-Stage Thermal Co-Evaporation: A Real-Time X-Ray Diffraction and Fluorescence Study, H. Rodriguez-Alvarez, A. Weber, J. Lauche, C. A. Kaufmann, T. Rissom, D. Greiner, M. Klaus, T. Unold, C. Genzel, H.-W. Schock and R. Mainz

PUSHING THE DOOR OPEN FOR SOLID-STATE PHYSICS

A group led by Dr. Martin Beye and Prof. Alexander Föhlisch has shown that X-ray measurements of solids can also exploit **non-linear physical effects**. Until now, this had only worked with laser light.

Basic physical research would be inconceivable without the plethora of X-raying methods available nowadays. With their research, the two scientists from Helmholtz-Zentrum Berlin (HZB) have opened up yet another type of application. Their results may very well influence the design of future X-ray sources. So-called non-linear effects are the basis of all laser physics, but have always seemed unusable for X-ray experiments. The physics behind all existing X-ray methods exploits linear effects only. That is to say, when an X-ray beam strikes a specimen, each light particle, or photon, in the beam acts alone.



On a silicon crystal, the researchers have shown how inelastic X-ray scattering (green light) can be amplified, where a frequency shift takes place. The exact colour emitted (red light) can be correlated very precisely with the structural properties of the material under study.

It is different with lasers. The energy and power density of the incident laser light can become so high that the photons work together, whereupon non-linear effects occur as they interact with the material. This has the result of materials greatly amplifying specific colours in the light. The upshot is that you can shine green light on a crystal and find that it emits red light instead. The exact colour emitted can be correlated very precisely with the structural properties of the material under study. Performing experiments at the short-pulse source FLASH at DESY in Hamburg, Alexander Föhlisch and his group have now demonstrated that the same effects can also be achieved with soft X-rays and that even solids are accessible to this measuring principle.

Photons amplify each other

"The efficiency of inelastic scattering processes with soft X-rays is normally poor," explains Martin Beye, first author of the paper. "With our experiment, we show how inelastic X-ray scattering can be cleverly amplified. Similarly to in a laser, all photons work together and mutually reinforce each other. That way, we obtain a very high measurement signal." With these kinds of set-ups at X-ray sources, efficient inelastic X-ray scattering processes could one day be used for analysing and interpreting extremely fast processes like the breaking and formation of chemical bonds, excitements in quantum materials (e.g. superconductors) and ultrafast switching processes, to name a few.

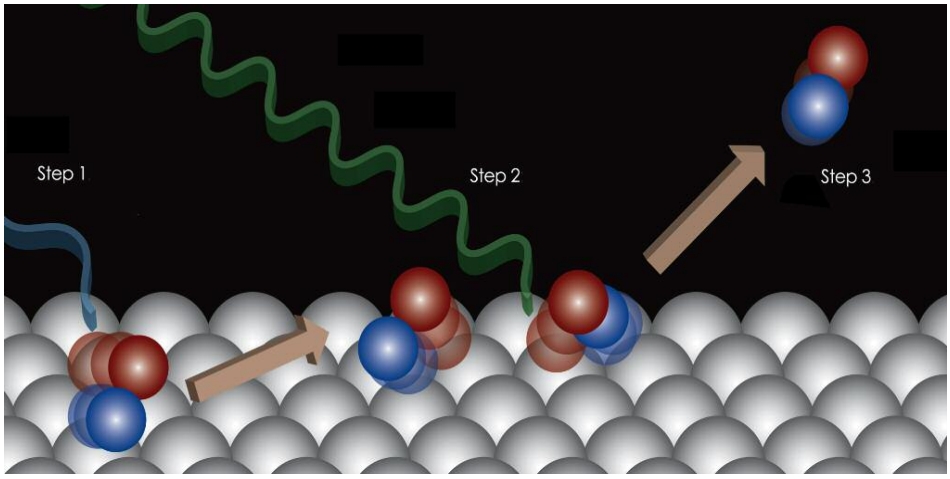
"Present X-ray sources are not at all optimised for the use of stimulated inelastic scattering," Alexander Föhlisch says. "From the new results, we know we can indeed exploit non-linear effects in soft X-rays. To do so, we need photon sources that can deliver short light pulses in rapid succession. This would have to be taken into account in the development of future photon sources." *ih*

Nature 501, 191–194 (12 September 2013), (doi:10.1038/nature12449): Stimulated X-ray emission for materials science, M. Beye, S. Schreck, F. Sorgenfrei, C. Trabant, N. Pontius, C. Schüßler-Langeheine, W. Wurth and A. Föhlisch

GAS CONVERSION IN THE CATALYTIC CONVERTER

On the **free-electron laser LCLS in Stanford**, an international group of scientists supported by HZB has observed for the first time in real time how carbon dioxide is formed on the surface of a catalyst. The researchers have thus explained one of the substeps in this important reaction.

Carbon monoxide is an odourless, invisible, toxic gas that is produced, among other things, from burning fuel. A suitable catalytic converter can ensure that carbon monoxide molecules react with oxygen in the air to produce the non-toxic gas carbon dioxide. So far, however, only the rough details of this catalytic process have been understood. "Catalysts are used in so many industrial chemical reactions that it is well worthwhile taking a closer look at them. That is what we have now done here, using an elementary process as an example," says Martin Beye of the institute "Methods and Instrumentation for Synchrotron Radiation Research", who was involved in the study.



First, the CO molecules were detached from the crystalline surface of the ruthenium catalyst using conventional laser pulses (blue), after which the researchers could observe using X-ray pulses on the LCLS (green) that these molecules remain close to the surface over a substantial period of time and can only move parallel to it. Only after a certain time (step 3) do the CO molecules completely escape from the surface.

One-third of the CO molecules did not fly away

The researchers studied how carbon monoxide molecules disconnect (desorb) from a ruthenium surface. Ruthenium is a metal that can act as a catalyst similar to platinum. In the first step, they fired conventional laser pulses at the surface of the ruthenium crystal to detach the CO molecules. Using ultra-short, high-intensity X-ray flashes at the free-electron laser LCLS at SLAC, Stanford, they then took snapshots from which they could deduce how the CO molecules come away from the catalyst surface. They observed that about one-third of the CO molecules did not immediately fly away from the surface as expected, but instead were "held captive" just above the surface. Aided by computer simulations, the measurements showed that weak bonds arise between the CO molecules and the catalyst surface. These weak bonds prevent the molecules from flying off, but they can still move freely parallel to the surface. Such weakly bound, activated states could play an important role in catalytic processes, the researchers believe. Their results were published in the journal Science.

Participants in the international collaboration were researchers from the Center for Free-Electron Laser Science at DESY, European XFEL, University of Hamburg, HZB, Fritz Haber Institute, University of Potsdam, Stockholm University, Technical University of Denmark, SLAC National Accelerator Laboratory and Stanford University. "Observing a reaction like this in real time is the dream of every chemist. We never expected to observe such weakly bound states; that was really a surprise," says Anders Nilsson, main author of the work, of Stockholm University and SLAC. *arö*

Science, Vol. 339, no. 6125, pp. 1302-1305; (DOI: 10.1126/science.1231711): Real-Time Observation of Surface Bond Breaking with an X-ray Laser, Martina Dell´Angela et al.

CONTROLLED CRYSTAL FORMATION

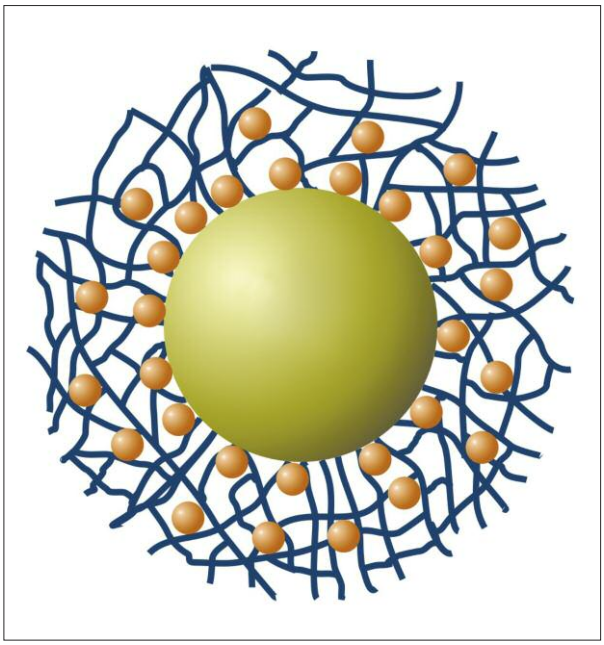
Scientists at HZB have managed to trigger the **formation of titanium dioxide nanoparticles** in a network of polymers at room temperature. By controlling the process, the particles can be manufactured for targeted applications.

Tiny particles of titanium dioxide are used in everyday products such as paint, toothpaste and sun cream, where they reflect the light or act as an abrasive. Yet as the particles become smaller, their properties start to change, where crystalline titanium dioxide nanoparticles even behave as catalysts: excited by the UV component in sunlight, they break down harmful substances or facilitate other desirable reactions. Chemists working with Dr. Katja Henzler of the HZB Institute "Soft Matter and Functional Materials" have discovered a synthetic pathway for producing such nanoparticles in a network of polymers at room temperature. By studying them at the Berlin synchrotron radiation source BESSY II, they proved that these nanoparticles are crystalline. This represents significant progress in the synthesis of so-called "polymeric nanoreactors", where nanoparticles have so far had to be heated to high temperatures to cause them to crystallise.

Novel combination of experiments

The "polymeric nanoreactors" from Katja Henzler's group consist of a polystyrene core enveloped by PNIPAM chains. The chemists added these polymeric structures to an ethanol-based solution. Upon adding a titanium compound, tiny titanium dioxide particles formed. These deposited into the PNIPAM network, which kept them at set distances and thus prevented the nanoparticles from sintering into larger particles. The chemists were able to control the speed of this process and – as shown in the studies at BESSY II – were accordingly able to influence the quality of the nanocrystals thus formed.

Using a novel combination of X-ray microscopy and spectroscopy (NEXAFS-TXM, U41-SGM) at BESSY II, Henzler and her colleagues in the microscopy group demonstrated that the embedded nanoparticles are distributed very evenly over the polymeric nanoreactors. They studied their samples in an aqueous environment, meaning they were able to study them without the typical desiccation step which can lead to artefacts. Their results show that the nanoparticles are crystalline, in that the TiO2 molecules sit at geometrically ordered lattice sites as they would in larger particles as well. "The nanocrystals have a tetragonal anatase structure, and this crystalline structure is important for their catalytic activity to unfold. Our new method also allows us to control the quality of the synthetic particles, meaning we can optimize the particles for different, specific applications," Katja Henzler says.



Crystalline titanium dioxide particles about 6 nanometres in diameter form out of solution in the polymer network around the polystyrene core (PS), even at room temperature.

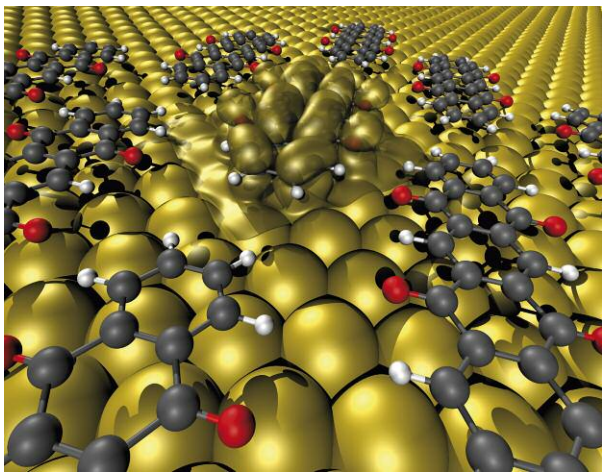
arö

Nano Lett., 2013, 13 (2), pp 824–828 (DOI: 10.1021/nl3046798): Electronic Structure of Individual Hybrid Colloid Particles Studied by Near-Edge X-ray Absorption Fine Structure (NEXAFS) Spectroscopy in the X-ray Microscope, K. Henzler, P. Guttmann, Y. Lu, F. Polzer, G. Schneider and M. Ballauff

GOOD CONNECTIONS

An international research group has identified which molecular properties lead to successful contact between carbon compounds and metal. Their success could bring further improvements to **organic electronics**.

Organic electronics is already used in the displays of smart phones nowadays and promises many more interesting products in future such as flexible luminescent films that could replace light bulbs or solar cells that convert sunlight to electricity. One of the problems so far is getting the active organic layer to connect solidly with metal contacts. Organic molecules are often used for this purpose as well. Nevertheless, it has never been possible to predict exactly which molecules will actually fulfil this task. Essentially, the only way to identify them was by trial and error. An international group of scientists working with Dr. Georg Heimel and Prof. Dr. Norbert Koch of HZB and of Humboldt-Universität has identified a set of properties which all successful molecules have in common. Their results could help improve the contact layers between



The organic compounds studied come into contact with the atoms of the metal surface through their "oxygen arms". This changes their electronic properties.

metal electrodes and active material in organic components in a targeted manner.
"We have been working for several years on this question, and have now gained a coherent picture using a combination of different measuring techniques and theoretical calculations," says Georg Heimel. The researchers systematically studied molecules whose backbone consists of a series of aromatic carbon rings. The candidates differed in just one detail: the number of oxygen atoms extending from this backbone. They applied these selectively modified molecules onto the typical contact metals gold, silver and copper.

Mediator properties identified

Using photoelectron spectroscopy (UPS and XPS) at the synchrotron radiation source BESSY II of HZB, they were able to measure the chemical bonds between the metal surface and organic molecules, as well as the energy levels of the conductive electrons. Colleagues from the University of Tübingen determined the exact distance of the molecules from the metal surface using X-ray standing wave measurements, which they performed at the synchrotron radiation source ESRF in Grenoble.
It turned out that upon close contact of the "oxygen arms" with the metal surfaces, the inner structure of the studied molecules changed in such a way that they lost their semiconducting properties and assumed the metallic properties of the substrate. Despite similar conditions, the "naked" backbone molecule did not exhibit this effect. From observing which of the studied molecules changed so drastically upon which metal, the researchers were able to derive a set of general rules. "We now have quite a precise understanding of how molecules should look and what properties they must contribute for them to mediate well between an active organic material and a metal, or in a sense to form a soft metallic contact," Heimel announces.

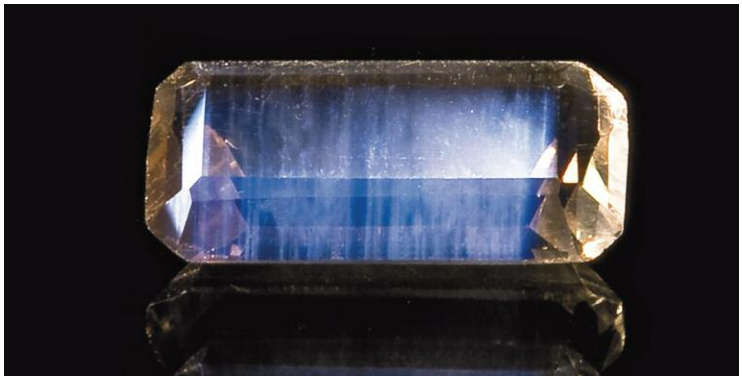
arö

Nature Chemistry, Volume 5, Issue 3, pp. 187-194 (2013) (DOI: 10.1038/nchem.1572): Charged and metallic molecular monolayers through surface-induced aromatic stabilisation; G. Heimel, S. Duhm, I. Salzmann, A. Gerlach, A. Strozecka, J. Niederhausen, C. Bürker, T. Hosokai, I. Fernandez-Torrente, G. Schulze, S. Winkler, A. Wilke, R. Schlesinger, J. Frisch, B. Bröker, A. Vollmer, B. Detlefs, J. Pflaum, S. Kera, K.J. Franke, N. Ueno, J.I. Pascual, F. Schreiber and N. Koch

REDISTRIBUTION OF ATOMIC NUCLEI OBSERVED IN SANIDINE

Mineralogists have studied the heat-related changes in **sanidine crystals** from various geographical regions using neutrons at HZB. The experimental facilities at HZB gave them a unique insight.

Mineralogists have long considered the sanidine crystals found near Volkesfeld in the Eifel to be special. The mineral may not be valuable or rare, but the crystals from Eifel are often quite long, at 20 to 30 centimetres, and often nigh perfect, which is why they are occasionally used in jewellery. Defects in the crystalline structure of their surface give them a grey-yellowish colour. Unlike many other sanidines, however, those from Volkesfeld can be "healed" especially quickly and gently by leaving them for a few hours in an oven several hundred degrees hot. Having studied this process for his doctoral thesis using neutrons from BER II, HZB researcher Johannes Kähn has doubts about the prevailing explanation for the Volkesfeld crystals' rapid healing.



Blue sanidine variety. After a while, the crystals display defects that can be "healed" with high temperatures. HZB researcher Johannes Kähn investigated exactly what happens during the process.

In close collaboration with crystal physicist Jürgen Schreuer of Ruhr-Universität Bochum (RUB), the HZB researcher analysed sanidines from five other regions in Eifel and from Madagascar in addition to the samples from Volkesfeld. To do so, he subjected the crystals to varying durations of treatment at temperatures between 600 and 1050 degrees Celsius, studying each of the samples before and after with neutron beams. Contrary to his expectation, he detected no major differences in the healing process between the different types of sanidine.

The illusion of quick-healing sanidine

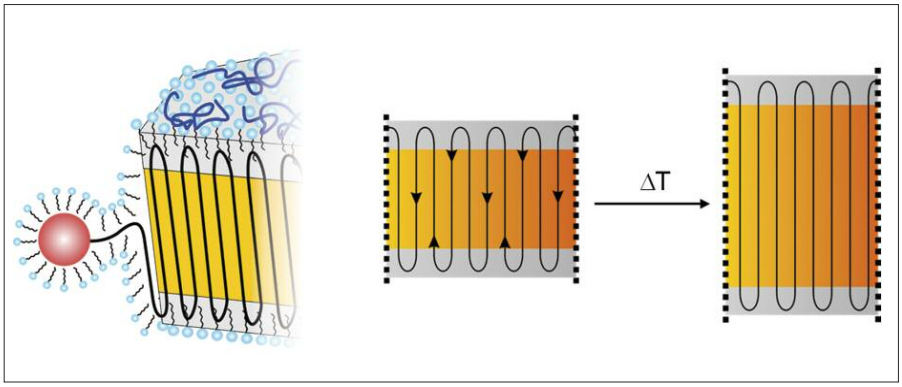
These results could well be due to the experimental method. Neutron beams namely "light up" the atomic nuclei. Sanidine consists of adjacent, three-dimensional tetrahedral figures composed of four equilateral triangles. At each of their four corners is an oxygen atom. Three-quarters of these pyramids possess a central silicon atom, while the remaining one-quarter possess an aluminium atom. As a sanidine crystal first forms, the aluminium atoms tend to be distributed relatively evenly at first. The crystal, however, comprises two slightly different types of tetrahedron where the aluminium fits into one type better than the other. Over time, the aluminium atoms therefore become concentrated in the more favourable pyramids. Heating the crystals causes the aluminium to distribute itself evenly again over the two types of tetrahedron.

The neutron beams of BER II distinguish the aluminium from the silicon nuclei very clearly, so Johannes Kähn was essentially able to observe this healing process directly. Curiously, in his experiments, the aluminium atoms did not redistribute throughout the Volkesfeld sanidines any faster than throughout the crystals from the other regions. Researchers had namely observed such a difference in earlier measurements using X-rays. This observation, however, was based on the electron clouds and not the atomic nuclei. Yet aluminium and silicon clouds are hard to distinguish under X-ray light. By contrast, the structures of the crystals show up excellently under X-rays. It is from this that the researchers then calculated the distribution of aluminium and silicon atoms. "Perhaps there is a slight inaccuracy in this calculation," Johannes Kähn speculates. That could create the illusion of faster healing in the Volkesfeld sanidines. Unfortunately, such an effect has not been detected using neutron beams so far. This shows, once again, how important it is to use the right measuring techniques for different scientific disciplines. *rk*

NEW PROPERTIES FROM AN IDEAL ALIGNMENT

Polyethylene is a plastic found in many household objects. Using a novel catalyst, a research group led by Prof. Dr. Matthias Ballauf has successfully synthesised an **ideal nanocrystal** out of this plastic.

Converting materials from an unordered (amorphous) molecular structure into a crystalline form is a common quest of chemists and materials scientists. Many substances only possess the desired properties when they are crystalline. Accordingly, researchers are keen to identify new physical principles underlying the transition from amorphous to crystalline form.



A water-soluble Ni(II) catalyst allows the polymerization of ethylene in aqueous solution. The illustration shows how the newly created parts of the PE chain are incorporated into the growing crystal. The amorphous areas act in the ideal nanocrystal like deflection pulleys that reverse the direction of the chains by 180 degrees.

Researchers working with Prof. Dr. Matthias Ballauff of the HZB Institute of Soft Matter and Functional Materials have identified such physical effects for the plastic polyethylene. In collaboration with colleagues from Bayreuth and Constance, they have developed a new, water-soluble catalyst that directly polymerises the small ethylene molecule into long-chain polyethylene in aqueous phase. Normally, such long-chain molecules exist in partially crystalline form. Specifically, they consist of lamellar polyethylene crystals covered with a layer of amorphous polyethylene. These amorphous phases exhibit a series of imperfections, like tangled knots.

Clever synthetic process avoids imperfections

In the newly synthesised "ideal nanocrystal", however, the amorphous areas act as deflection pulleys that reverse the direction of the chains in the crystal by 180 degrees. The researchers achieved this structure in a clever synthetic process: during polymerisation in aqueous phase, the newly created parts of the molecular chain are immediately captured by the growing crystal so that no imperfections such as tangling can arise in the amorphous areas.

The researchers confirmed this using X-ray diffraction and cryogenic transmission electron microscopy (TEM). This method resolves to about one nanometre and is especially suitable for studying the minutest structures in microemulsions and colloidal solutions. For their cryo-TEM measurement, the scientists produced a thin film of polyethylene nanocrystals out of an aqueous suspension, which they then flash froze using cryogenic liquid ethane. This produced a glass-like, solidified water modification, allowing them to analyse the encased polyethylene nanocrystals under the electron microscope. They additionally performed X-ray studies of these suspensions using small-angle X-ray scattering (SAXS).

Matthias Ballauff stresses the importance of this combination of methods: "Only by combining microscopy and scattering can such complex systems be analysed to a precision that neither method can offer on its own." The two methods combined also proved that the nanoscale polymer crystals were in fact perfect. The crystalline nanostructure lends the plastic new properties and could be of interest in the production of novel coatings, for example.

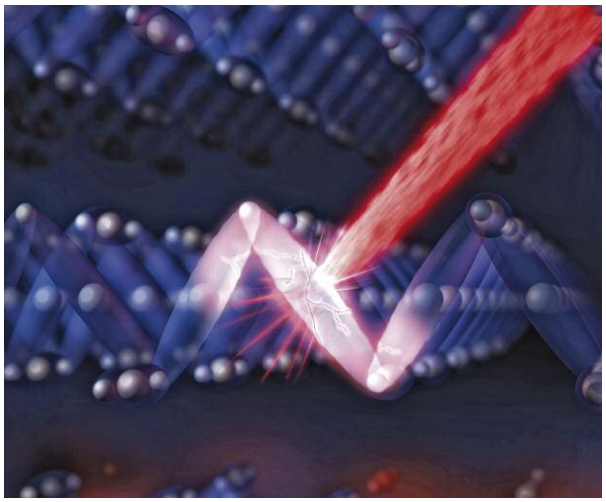
ih

J. Am. Chem. Soc., 2013, 135 (31), pp 11645–11650 (DOI: 10.1021/ja 4052334): Ideal Polyethylene Nanocrystals, A. Osichow, C. Rabe, K. Vogtt, T. Narayanan, L. Harnau, M. Drechsler, M. Ballauff and S. Mecking

PICOSECOND-FAST SWITCHES

An international research group in which HZB scientists were instrumentally involved has shown that **oxide materials** switch considerably faster than semiconductors. They have observed the process of an iron oxide switching between the non-conducting and conducting state at unprecedented precision.

Materials that can be switched to be either conducting or insulating are considered highly suitable for future electronic components such as transistors. The iron oxide known as magnetite is the most well-studied representative of this class of materials. It acts as an insulator at low temperatures and becomes conductive at high temperatures. This switching process, however, happens so fast that no one has ever truly known what goes on at the atomic level.



An optical laser flash (red) disrupts the electronic order (blue) in magnetite, switching the material's state from insulating to conducting within a trillionth of a second.

In an experiment at the American source of ultra-short X-ray flashes, LCLS of the national laboratory SLAC, an international research group has now managed to freeze the switching process in a kind of shortest-possible slow motion. In doing so, they revealed that the transition takes place in two steps: "In a first step, conductive islands form in the insulating material. Then it takes less than a picosecond (a trillionth of a second) before the atoms reorganise to form a completely metallic lattice," explains Christian Schüßler-Langeheine of Helmholtz-Zentrum Berlin.

Time-resolved measurement in the extreme range

Schüßler-Langeheine and his group performed the groundwork for the SLAC experiment at the electron storage ring BESSY II. Working from the information they obtained, the experiment was then designed and successfully performed at SLAC.

For the experiment in California, the researchers cooled the magnetite to minus 190 degrees Celsius and then fired infrared laser light onto it. This additional energy triggered the switching process. They immediately followed with an X-ray laser pulse, by which they could observe the switching process as if with a strobe lamp. Only very few photon sources in the world allow this kind of time-resolved measurement at picosecond intervals.

"At HZB, we are researching into materials for faster and more energy-efficient electronics," says Christian Schüßler-Langeheine. "In this experiment, we saw how extremely fast a switch made of an oxide material like magnetite can be. That makes oxides exciting alternatives to the currently popular semiconductors, especially materials that exhibit metal–insulator transitions even at room temperature."

International cooperation

The research project involved colleagues from SLAC and Stanford University, CFEL and the University of Hamburg, the Universities of Amsterdam, Cologne, Potsdam, Regensburg, the Max Planck Institute CPfS in Dresden, the European X-ray pulse sources ELETTRA in Trieste and XFEL in Hamburg, the Advanced Light Source in Berkeley and the Swiss Paul Scherrer Institute. The samples were prepared at Purdue University.

ih

Nature Materials 12, 882–886 (2013) (doi: 10.1038/nmat3718): Speed limit of the insulator–metal transition in magnetite, S. de Jong, R. Kukreja, C. Trabant, N. Pontius, C. F. Chang, T. Kachel, M. Beye, F. Sorgenfrei, C. H. Back, B. Bräuer, W. F. Schlotter, J. J. Turner, O. Krupin, M. Doehler, D. Zhu, M. A. Hossain, A. O. Scherz, D. Fausti, F. Novelli, M. Esposito, W. S. Lee, Y. D. Chuang, D. H. Lu, R. G. Moore, M. Yi et al.

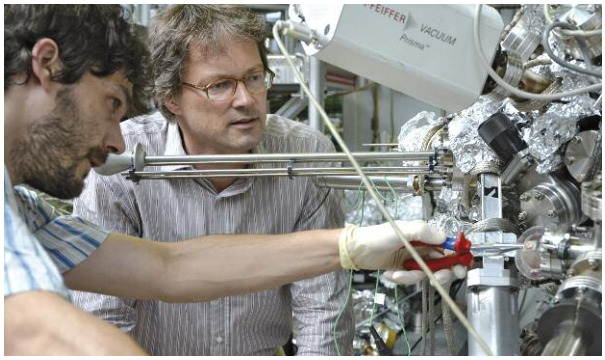
CONTROLLING ELECTRON SPINS WITH LIGHT

Topological insulators are a highly promising research field. A group at HZB has discovered how to modify the physical properties of electrons in these materials using light.

Discovered only a few years ago, the material class of topological insulators has gained much attention for their extraordinary properties: they behave as electrical insulators inside, but form metallically conductive states on their surface. This behaviour emerges largely from the spin of their electrons, i.e. the electrons' rotation around their own axes. On the material surface, the electrons' direction of spin is namely directly coupled with their direction of motion, and that leads both to high stability of the metallic state and to particularly low-loss electrical conductivity. Topological insulators are accordingly treated as exciting and promising candidates for novel components in information technology. The Deutsche Forschungsgemeinschaft (DFG) has therefore initiated the focus programme "Topological Insulators: Materials – Fundamental Properties – Devices", to further our physical understanding of the surface states in topological insulators.

Experiments with light at varying energies

An especially innovative approach is to use light to manipulate the spins of surface electrons in components of this kind. HZB scientist Prof. Dr. Oliver Rader, coordinator of the DFG focus programme, and his group have discovered what influences can be used to manipulate electron spins on the surfaces of topological insulators by performing experiments using light at varying energies and wavelengths.
They used spin-resolved photoelectron spectroscopy at the synchrotron ring BESSY II to study the well-known topological insulator bismuth selenide (Bi_2Se_3) and gained astonishing insights: they discovered it makes a substantial difference whether the electrons on the material surface are excited with circularly polarized light in the vacuum ultraviolet range (50–70 electron volts) or with ultraviolet laser light (6 electron volts).
In their experimental set-up they demonstrated that at the high energies typically used at the synchrotron, they can measure the electron spins without changing them. "When excited with 50 electron volts, the emitted electrons exhibit the spin texture typical of topological insulators," explains Dr. Jaime Sánchez-Barriga, who made the measurements.



Dr. Jaime Sánchez-Barriga and Prof. Dr. Oliver Rader preparing their experiments with light at varying energies at the synchrotron ring BESSY II.

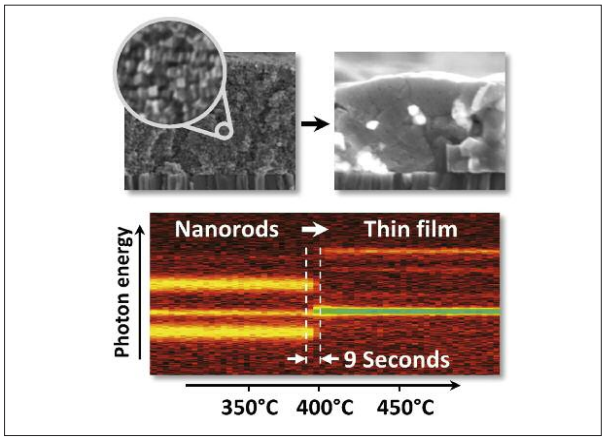
"The electron spins here in the surface plane run in a circle, much like on a road sign for a roundabout." This is the ground state of the electrons in the surface of topological insulators.
When excited using low-energy, circularly polarized photons (6 eV), on the other hand, the electron spins rotated entirely out of the plane. In fact, they even assumed the spin direction dictated by the clockwise or anticlockwise polarization of the light. That means the spin can be manipulated in a targeted manner by carefully choosing the type of light. The scientists were even able to explain this entirely different behaviour at different energy strengths, tracing it back to symmetry characteristics. This result delivers important insights into how spin currents can be produced losslessly in topological insulators, Rader is convinced. And that in turn is important for the development of so-called optospintronic components, which could enormously increase data processing and storage speeds. *tm*

Physical Review X 4, 011046 (doi: 10.1103/PhysRevX.4.011046): Photoemission of Bi_2Se_3 with Circularly Polarized Light: Probe of Spin Polarisation or Means for Spin Manipulation?; J. Sánchez-Barriga, A. Varykhalov, J. Braun, S.-Y. Xu, N. Alidoust, O. Kornilov, J. Minár, K. Hummer, G. Springholz, G. Bauer, R. Schumann, L. V. Yashina, H. Ebert, M. Z. Hasan and O. Rader

FROM NANOROD CARPET TO THIN FILM FOR SOLAR CELLS

Research teams from HZB and the University of Limerick, Ireland, have found a new way to produce **thin films of polycrystalline kesterite** at low temperature. This could make solar cells substantially cheaper to produce.

Kesterite semiconductors are regarded as promising alternatives to chalcopyrite solar cells ($Cu(In,Ga)Se_2$), which already exceed 20 percent efficiency in the laboratory. Kesterites have similar physical properties to chalcopyrite semiconductors, but can be made without the relatively scarce elements indium and gallium. For their experiments at HZB, the researchers started with a 'carpet' of nanorods featuring an ordered wurtzite crystal structure. Chemists from the University of Limerick had produced these highly ordered layers in chemical processes that yielded wurtzite nanorods with exactly the same composition as the kesterite Cu_2ZnSnS_4.



The transition from a layer of densely packed nanorods (top left) into a polycrystalline semiconductor thin film (top right) can be observed in realtime using in-situ X-ray diffraction. In the bottom image, the intensity of the X-ray signals is colour-coded. Detailed analysis of the signals reveals that the transformation from nanorods to kesterite crystals takes only 9 to 18 seconds.

Using real-time X-ray diffraction on the EDDI beamline at BESSY II, the HZB physicists working with Roland Mainz and Thomas Unold revealed how the crystalline structure of these rods transforms into a stable kesterite structure upon heating. Specifically, heating brings about a solid-state phase transition from the metastable wurtzite phase into the stable kesterite phase. When this happens, the macroscopically arranged nanorods transform into thin kesterite films featuring grains almost micrometres in size. It was not the temperature itself that was important in their process, but rather the rate of heating: The faster the wurtzite rods were heated, the larger the grains became. Accordingly, they were able to choose parameters that yielded kesterite films with almost micrometre-sized grains that could be used in thin-film solar cells.

"It is interesting to see how the complete formation of the kesterite film happens so fast, and that rapid grain growth is simultaneously triggered," Mainz says. Also, the faster the samples are heated, the larger the grains become. "With slow heating, the transition from wurtzite to kesterite already starts at a lower temperature, where many small grains form instead of fewer larger ones. More defects also arise when this happens. When heated faster, there is no time for this to happen; the transition only takes place when the temperature is already high, where a faultless structure forms straight off," Mainz concludes.

Interplay of grain growth and phase transition

Comparing how the phase transition evolves during slow and fast heating reveals not only that the phase transition triggers grain growth, but also that grain growth actually accelerates the phase transition. The HZB physicists have developed a model that can explain this observation and, by making model calculations, have verified its agreement with the measured data. The work points towards a new pathway for fabricating thin microcrystalline films of semiconductor nanostructures without elaborate and costly vacuum technology. Mainz believes the new method could also be of interest for fabricating micro- and nanostructured photoelectric components as well as for semiconductor films made of other materials. *arö*

Nature Communications, Vol. 5, 2013 (doi:10.1038/ncomms4133): Phase-transition-driven growth of compound semiconductor crystals from ordered metastable nanorods, R. Mainz, A. Singh, S. Levcenko, M. Klaus, C. Genzel, K. M. Ryan and T. Unold

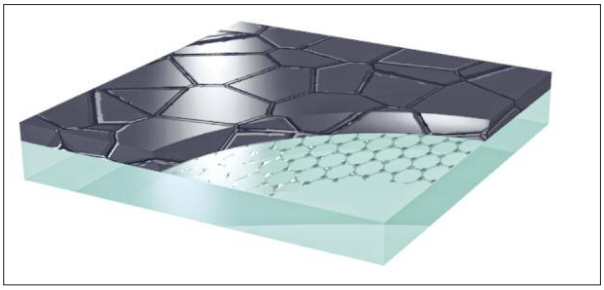
GRAPHENE STAYS GRAPHENE EVEN UNDER A LAYER OF SILICON

HZB scientists Dr. Marc Gluba and Prof. Norbert Nickel have experimentally shown that graphene retains its special properties even when covered by a thin film of silicon. This opens up entirely new possibilities for **thin-film photovoltaics**.

Graphene is extremely conductive and completely transparent to light, while also being cheap and non-toxic. That makes it perfect for use in solar cells as a transparent contact layer that will conduct electric current without reducing incident light – at least in theory. Whether this actually works in the real world, however, has long been debated, since "ideal" graphene – a free-floating, flat honeycomb structure existing as a single layer of carbon atoms – does not exist: interactions with neighbouring films, the argument goes, can alter graphene's behaviour drastically.
Marc Gluba and Norbert Nickel of the HZB Institute for Silicon Photovoltaics conducted experiments to find out once and for all how graphene behaves when covered by a thin film of silicon. "We studied how the conductive properties of graphene would change if we incorporated it into a stack of layers like in a thin-film silicon solar cell. We were surprised to discover these properties changed only marginally as a result," Marc Gluba reports.

Graphene detectable even after silicon crystallisation

For this, the researchers produced graphene on a copper foil, transferred it onto a glass substrate and then deposited a thin film of silicon on top of it. They studied two popular variants used in modern thin-film silicon technologies: first, they studied a sample with an amorphous silicon layer in which the silicon atoms were unordered as in a solidified melt. Second, they studied how a typical crystallisation process, which causes the unordered silicon to transform into its crystalline phase, would affect the properties of the graphene.



The graphene layer is only one atom layer thick (0.3 ångströms or 0.03 nanometres), yet its charge carriers can move with extreme freedom within it. These properties remain unchanged even when the graphene layer is coated with amorphous or polycrystalline silicon.

Heated to several hundred degrees Celsius, the structure of the covering layer changed completely, but the graphene was still detectable beneath it after the process. "We had not expected this, but our results show that graphene stays graphene even under a layer of silicon," says Norbert Nickel. Hall-effect mobility measurements showed that the mobility of charge carriers in the embedded graphene layer is roughly 30 times greater than in conventional zinc oxide contact layers. "Yet it is still very difficult to combine this contact layer, which is only one atom layer thick, with external contacts. We still have to work on that," Gluba explains. "Our thin-film technology colleagues are already pricking up their ears and wanting to incorporate it," says Nickel. The researchers performed their measurements on samples only a few square centimetres in size. Yet the graphene-coating technique can in principle be scaled-up to coat larger areas, making the results of serious interest for industry as well. *arö*

Appl. Phys. Lett. 103, 073102,2013, (doi: 10.1063/1.4818461): Embedded graphene for large-area silicon-based devices; M. A. Gluba, D. Amkreutz, G. V. Troppenz, J. Rappich and N. H. Nickel

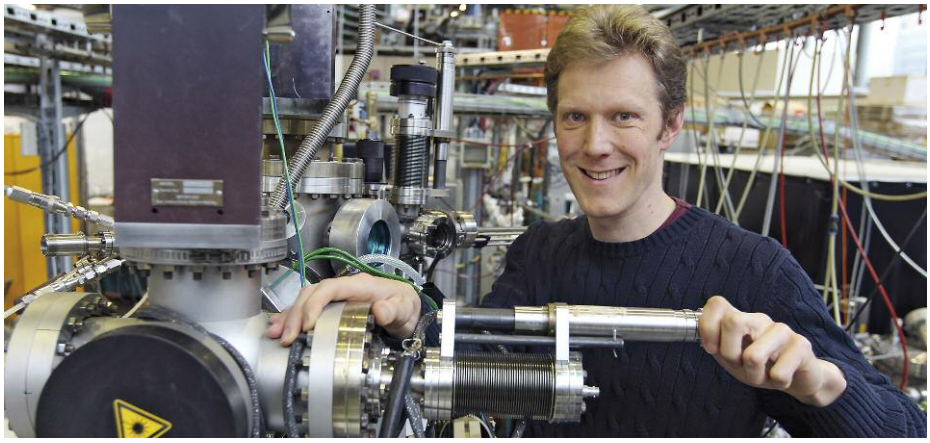
HZB INVOLVED IN BMBF INITIATIVE

In the scope of its initiative "Materials Research for the Energy Turnaround", the Federal Ministry for Education and Research (BMBF) is funding 17 out of 290 submitted applications, including an application from HZB. This provides additional means for developing novel materials for solar hydrogen production and investigating the role of defects.

RAPID DEMAGNETISATION BY SPIN TRANSPORT

Ultra-short laser pulses can demagnetise a ferromagnetic layer in a flash. Physicist Dr. Andrea Eschenlohr and fellow researchers have shown that it is apparently not the light itself that causes the demagnetisation.

It has been known since 1996 that an ultra-short laser pulse can demagnetise a ferromagnet as quick as a flash. Yet it has never been fully understood how this demagnetisation works. Physicist Dr. Andrea Eschenlohr and colleagues from HZB and the University of Uppsala in Sweden studied this phenomenon in their research. They fired extremely short laser pulses of a mere hundred femtoseconds (10^{-15} s) duration at two different layer systems: one sample consisted of a thin ferromagnetic layer of bare nickel, while the other sample was a similar nickel layer covered by a non-magnetic layer of gold. This gold layer, although only 30 nanometres (10^{-9} m) thick, absorbed most of the laser light, allowing almost no light to reach the nickel. And yet, instants after irradiation with the laser pulse, the magnetisation of the nickel layer promptly decayed in both samples, whereas this happened after a split-second temporal delay in the gold-coated sample. The researchers observed this by taking measurements with femtosecond-long pulses of circular polarised X-rays, which they performed on the femtoslicing beamline at the Berlin electron storage ring BESSY II, operated by HZB.



Dr. Christian Stamm, head of the experiment of Dr. Andrea Eschenlohr on the femtoslicing beamline at the electron storage ring BESSY II.

Selectively generating spin currents with laser pulses

"We were able to show experimentally that the ultrafast demagnetisation is not caused by the light itself, but rather by hot electrons created by the laser pulse," explains Andrea Eschenlohr. These excited electrons can move extremely rapidly over short distances such as through the ultra-thin gold coating. They transport their magnetic moment ("spin") with them into the ferromagnetic nickel layer, subsequently breaking down the existing magnetic order in the nickel. "We had actually hoped to see how we could use the laser pulse to influence the spins," head of the experiment Dr. Christian Stamm explains. "That we would directly observe how these spins migrate came as a complete surprise."
Laser pulses are therefore a means of creating "spin currents" in a targeted manner, where spin is transmitted instead of electric charge. This observation is relevant for spintronics research, where researchers develop new devices from magnetic layer systems that "calculate" with spins instead of electrons, enabling them to process and store information extremely rapidly while also saving energy. Dr. Andrea Eschenlohr worked at HZB until the end of 2012, where she obtained these results in the scope of her PhD work. Since January 2013, she has been working as a scientific associate at the University of Duisburg-Essen.

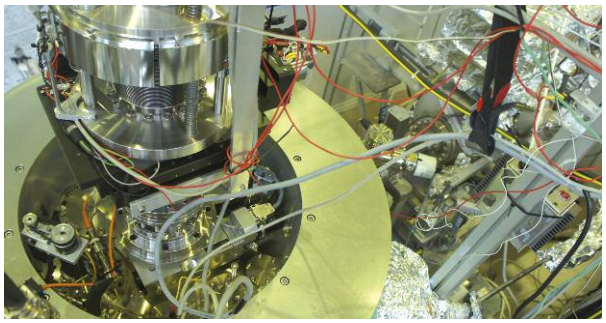
arö

Nature Materials 12, 332–336, 2013, (doi:10.1038/nmat3546): Ultrafast spin transport as key to femtosecond demagnetisation; A. Eschenlohr, M. Battiato, P. Maldonado, N. Pontius, T. Kachel, K. Holldack, R. Mitzner, A. Föhlisch, P. M. Oppeneer and C. Stamm

CONTROLLING MAGNETIC MOMENTS

Researchers at HZB have worked out how to manipulate the **physical characteristics of metal oxides** in a targeted manner, thus revealing new paths for the mechanisms of future information technologies.

In the quest for increasingly powerful storage media for use in information technology, physicists are creating and manipulating magnetic structures. Spintronics, as the field is called, exploits the magnetic properties of electrons and could even replace conventional electronics, which only makes use of electron charge. The challenge for science is to identify suitable materials, decipher their electronic and magnetic structure and then selectively control the associated physical properties and functionalities.
Whether and how the characteristics of atom-thin metal oxide nanostructures can be influenced was the topic of research in an experiment performed at HZB in cooperation with the Max Planck Institute of Solid-State Research in Stuttgart and the Quantum Matter Institute of the University of British Columbia, Vancouver. As suitable objects of



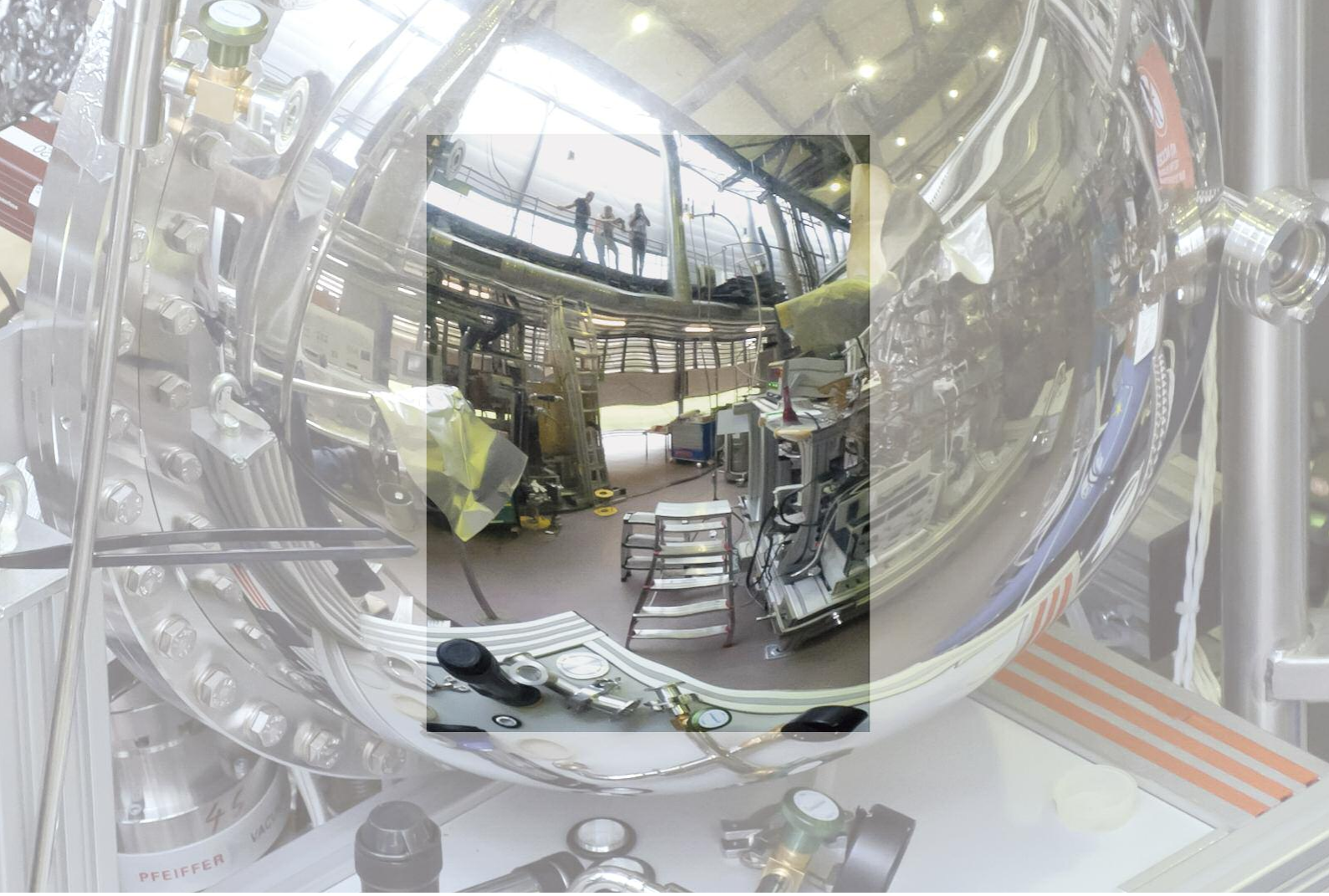
The researchers performed their experiments with lanthanum nickel oxide on the XUV diffractometer developed by HZB.

investigation, the researchers working with Dr. Alex M. Frano Perreira and Dr. Enrico Schierle identified rare-earth nickel oxides, which have some rather special physical properties: the complex interplay between different electronic degrees of freedom in these substances allows transitions between metallically conductive and highly insulating behaviour, which is accompanied by different magnetic and charge order states.
Such states can be manipulated in a targeted manner in nanostructures of these materials: lanthanum nickel oxide, for example, exhibits no magnetic properties in a large volume, but becomes magnetically ordered when it is only two atom layers thick. The researchers' challenge was to find out exactly what magnetic structures these atomic layers create – whether a ferromagnetic or an antiferromagnetic order exists, for example, and whether the material has a simple or a complex, spiral magnetic order.

X-ray scattering at BESSY II

The researchers performed their experiments on the XUV diffractometer developed by HZB and operated at the UE46_PGM1 beamline at BESSY II. Employing soft X-ray synchrotron radiation for resonant X-ray scattering, they were able to characterize these elusive nanostructures with high precision, making a significant contribution to our understanding of this phenomenon. The researchers were rewarded with answers to important questions: The experiment showed that magnetic structures and other macroscopic properties of the nickelates can be specifically tailored. "If you grow these extremely thin materials on a substrate, then the lattice constants of the substrate are never a perfect fit to the lattice constant that the material would develop by itself. That means you distort these materials ever so slightly due to the choice of the substrate and thereby influence the orbital occupancy and, with it, the direction of the magnetic moments," Dr. Schierle explains the method.
This insight opens up the unique opportunity of researching the potential of antiferromagnet-based spintronics. The aim is to "find the functionalities that allow you to switch the system from one stable state into another by making the simplest possible parameter changes. That is the prerequisite for it being useful for information storage processes," says Dr. Schierle. *tm*

Phys. Rev. PRL 111, 106804 (2013), (DOI: 10.1103/PhysRevLett.111.106804): Orbital Control of Noncollinear Magnetic Order in Nickel Oxide Heterostructures, A. Frano, E. Schierle, M.W. Haverkort, Y. Lu, M.Wu, S. Blanco-Canosa, U. Nwankwo, A.V. Boris, P.Wochner, G. Cristiani, H. U. Habermeier, G. Logvenov, V. Hinkov, E. Benckiser, E. Weschke and B. Keimer.



JOINT VENTURES

194 joint ventures with other scientific establishments had been hosted at HZB at the end of 2013. Of these, 75 were for research on renewable energies and 119 for research with photons, neutrons and ions.

Alongside the **Berlin Joint EPR Lab** (see page 44), HZB concluded cooperation agreements with FU Berlin on the establishment of three other joint labs: the Berlin Joint Laboratory for Quantum Magnetism (BerQuam), the Berlin Joint Laboratory for Non Equilibrium of Matter (BerNEM), and “Supramolecular Polymeric Materials”. The establishment of these joint labs promotes young talent with the joint appointment of one junior professor each.

Together with Humboldt University (HU Berlin), HZB is setting up the **graduate school Hybrid Materials for Efficient Energy Generation and Information Technologies**. This will be part of the Humboldt Graduate School (HGS). The school’s scientific focus will be on inorganic-organic hybrids for photovoltaics. In charge are Prof. Norbert Koch, who heads a joint research group of HZB with Humboldt University, and Prof. Joachim Dzubiella (HZB and HU Berlin).

BREAKTHROUGH IN SOLAR HYDROGEN PRODUCTION

Using a simple solar cell and a **metal-oxide photoanode**, researchers from HZB and TU Delft were able to store almost five percent of solar energy chemically in the form of hydrogen.

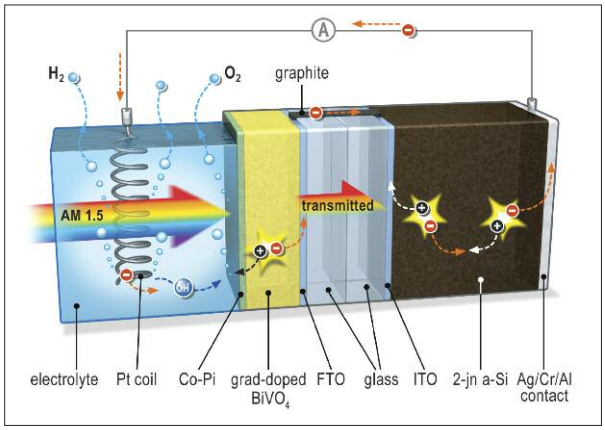
Working out how to store solar energy for those days devoid of sunshine is key to a sustainable energy future. Researchers working with Prof. Dr. Roel van de Krol, head of the HZB Institute for Solar Fuels, have made an important breakthrough with their experimental design. The solar cell they are using is of much simpler construction than the typical high-power cells comprising "triple junctions" of thin, amorphous silicon layers or expensive III-V semiconductors. The photoanode made from the metal oxide bismuth vanadate ($BiVO_4$) was simply spray-deposited onto a glass substrate – alternating with additional tungsten atoms – and coated with a low-cost cobalt phosphate catalyst.

"We have combined the best of two worlds here," says Roel van de Krol: "We exploit the chemical stability and the low cost of metal oxides, combine this with an excellent, yet very simple thin-film silicon solar cell, and obtain a cheap, highly stable and powerful cell." The experts have thus developed a simple system that can split water into hydrogen and oxygen using sunlight. Known as "artificial photosynthesis", this process can be used to store the energy from the sun chemically in the form of hydrogen. The relatively simple thin-film silicon cell is combined with a metal oxide layer that acts as a photoanode for the formation of oxygen. Only this photoanode comes into contact with the aqueous solution, protecting the sensitive silicon cell against corrosion.

Higher efficiencies are possible

In order to optimize the system even further, van de Krol and colleagues systematically studied the processes involved, from light incidence and charge separation to water splitting, in different metal oxides. "Theoretically, with a bismuth vanadate photoanode, the electrochemical cell ought to be able to reach efficiencies of up to nine percent," van de Krol announces. They have already solved one problem, for instance: by applying a low-cost cobalt phosphate catalyst, they managed to significantly accelerate the formation of oxygen at the photoanode.

The biggest challenge, however, was achieving efficient charge separation in the bismuth vanadate layer. Metal oxides may be stable and cheap, but their charge carriers tend to recombine too quickly before they can be used for splitting the water. Van de Krol and his colleagues discovered that incorporating additional tungsten atoms into the bismuth vanadate layer counteracts this effect. "It comes down to distributing these tungsten atoms optimally; then they create an internal electric field that prevents recombination," van de Krol explains. To achieve this, they sprayed a solution of bismuth, vanadium and tungsten onto a hot glass substrate. By alternating the tungsten concentrations with each spraying process, they produced an efficient photoactive metal oxide layer of about 300-nanometre thickness. "We determined that more than 80 percent of the trapped photons are actually used. That is truly a record for a metal oxide and was even physically unexpected," van de Krol reports. One of the next challenges will be scaling these systems up to square-metre magnitude to produce real-world quantities of hydrogen. *arö*



When light strikes the system, an electric voltage is created. The metal oxide layer acts as a photoanode, where oxygen forms. It is connected to the solar cell via a conductive graphite bridge (black). Because only the metal oxide layer comes into contact with the electrolytes, the rest of the solar cell remains protected against corrosion. A platinum coil serves as a cathode, where hydrogen forms.

Nature Communications (doi: 10.1038/ncomms3195): Efficient solar water splitting by enhanced charge separation in a bismuth vanadate-silicon tandem photoelectrode; F. F. Abdi, L. Han, A. H. M. Smets, M. Zeman, B. Dam and R. van de Krol

MATERIALS RESEARCH WITH SPECTROSCOPY

HZB and Freie Universität Berlin have established a joint laboratory where they can develop **electron-spin-resonance-based methods** for studying new materials and biological systems: the "Berlin Joint EPR Laboratory" (BeJEL).

The scientists at BeJEL are employing the latest generation of high-resolution and ultra-high sensitivity spectroscopic methods to study, among other things, materials for catalytic and photovoltaic applications. By analysing the physical-chemical processes taking place within solar cells, catalytic converters and proteins, for example, the researchers are contributing towards the development of higher-performance components for generating and storing renewable energies.

Opening ceremony for the common laboratory (left to right): Prof. Dr. Monika Schäfer-Korting, Prof. Dr. Robert Bittl, Prof. Dr. Klaus Lips, Prof. Dr. Thomas Risse and Prof. Dr. Anke Kaysser-Pyzalla.

Electron paramagnetic resonance (EPR), also known as electron spin resonance (ESR), is an especially promising spectroscopic technique for experiments of this kind: The efficiency of solar cells is often limited by defects at the atomic scale that arise during the manufacturing process – such as minute contaminations in the material that lead to defects during the formation of ultra-thin films for solar cells. These defects can be detected using electron spin resonance, after which the solar cell manufacturing process can be optimised.

Combined know-how

The new establishment is managed by Prof. Dr. Klaus Lips, head of the Energy Materials In-Situ Lab (EMIL) at HZB and chair of photovoltaic analytics at Freie Universität Berlin, as well as Robert Bittl, professor of experimental physics, and Thomas Risse, professor of physical and theoretical chemistry at FU Berlin. At the opening ceremony in February 2013, HZB scientific director, Prof. Dr. Anke Kaysser-Pyzalla, announced that the founding of BeJEL is an important step "by which we are intensifying our collaboration with FU Berlin. The combined know-how that we bundle in the new lab will significantly strengthen Berlin as an internationally leading hub in materials and energy research." The first vice-president of Freie Universität Berlin, Prof. Dr. Monika Schäfer-Korting, positively noted that the opening of the jointly run laboratory reinforces the cooperation between FU Berlin and Helmholtz-Zentrum Berlin: "This cooperation opens up new latitudes and perspectives in many respects for the Freie Universität," Schäfer-Korting said. As examples, she named the gain in research and teaching personnel, the joint recruitment of top researchers in international networks, joint projects and the promotion of young scientists. *hs*

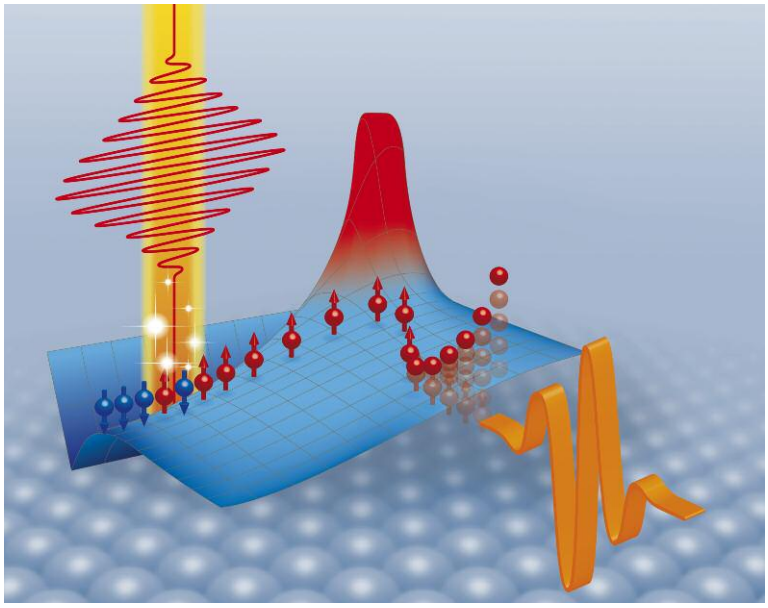
NEW JOINT LAB AT HZB

With the Fritz Haber Institute and the University of Darmstadt, the HZB Institute for Solar Fuels has established a joint lab for studying boundaries between metal oxide semiconductor compounds and electrolytes in order to improve electrocatalysis. For this, HZB has created two new postdoc positions.

ULTRAFAST PROCESSES IN MAGNETS

An international group has discovered a way to control spins at unprecedented speeds, namely at terahertz frequency. They did so using **femtosecond laser pulses**. These are exciting results for data processing and storage.

How rapidly can you switch electric power on and off? New ways of testing these limits were studied in magnetic materials by an international research group involving the Fritz Haber Institute, the Universities of Göttingen and Uppsala, Forschungszentrum Jülich and Helmholtz Zentrum Berlin. The scientists successfully produced and manipulated electric currents on a timescale of 100 femtoseconds – where one femtosecond is a millionth of a billionth of a second. The results could allow the design of new materials in which magnetic patterns can be stored at significantly higher speeds.



Excited by a femtosecond laser pulse (yellow), an ultrafast spin current occurs (red balls with arrow). It generates electromagnetic radiation in the terahertz frequency range (orange).

Elementary particles, many atomic nuclei and atoms with specific electron configurations exhibit a property called "spin", or the particle's rotation around its own axis. This property of electrons allows an alternative form of current control known as "spin electronics" or "spintronics" for short. The researchers produced a layer system only a few nanometres thick in which they could store and read out ultra-fast currents. Excited by a femtosecond laser pulse, they produce a so-called spin current. This spin current can be localized and stored by exploiting its special properties and its interactions with the metal in which it flows.

Once stored, a spin current can be converted into a conventional charge current

In their study, the scientists showed that the metal ruthenium makes for a good storage medium. By contrast, spins will simply flow straight through a layer of gold, for example. Once stored, the spin current can be converted into a conventional charge current. The current flow can be detected by the electromagnetic radiation it generates in the terahertz frequency range. "Only with these ultra-short current pulses lasting 100 femtoseconds can long-wavelength electromagnetic waves be produced in the terahertz range," says physicist Prof. Dr. Markus Münzenberg from Göttingen. "By using different materials such as ruthenium or gold, we can control the spectrum of the electromagnetic waves. We are currently working on actively influencing such a control."

Terahertz-frequency electromagnetic waves are of great interest for ultrafast information technology and for the development of novel light sources. They are also needed for precisely analysing complex crystals and molecules and are highly important for developing and producing pharmaceutical products.

hs

Nature Nanotechnology, 2013, (doi: 10.1038/nnano.2013.43): Terahertz spin current pulses controlled by magnetic heterostructures; T. Kampfrath, M. Battiato, P. Maldonado, G. Eilers, J. Nötzold, S. Mährlein, V. Zbarsky, F. Freimuth, Y. Mokrousov, S. Blügel, M. Wolf, I. Radu, P. M. Oppeneer and M. Münzenberg

NEW HELMHOLTZ INSTITUTE FOR RENEWABLE ENERGIES

Together with two partners, HZB has established the Helmholtz Institute Erlangen-Nürnberg for **Renewable Energies** (HI ERN).

The new Helmholtz Institute Erlangen-Nürnberg for Renewable Energies aims at improving the scientific bases for obtaining and storing renewable energies. Three scientific establishments – Friedrich Alexander University of Erlangen-Nürnberg (FAU), Forschungszentrum Jülich and Helmholtz Zentrum Berlin (HZB) – entered a cooperation agreement to this effect in August 2013. The Helmholtz Association is funding the new institute, which will employ 40 to 50 people in the medium term, with 5.5 million euros a year. Covered by this budget are, among other things, four professorships and two junior groups. The partners from Jülich, Berlin and FAU are working closely together on the appointments, where employee and student exchanges are also planned.

Cooperation partners (left to right): Prof. Dr. Jürgen Mlynek, President of the Helmholtz Association, Katja Hessel, State Secretary of the Bavarian State Ministry for Economy, Infrastructure, Traffic and Technology, Dr. Wolfgang Heubisch, Bavarian State Minister for Science, Research and Art, Joachim Herrmann, Bavarian State Minister of the Interior, Prof. Dr. Johanna Wanka, Federal Minister for Education and Research, Prof. Dr. Karl-Dieter Grüske, President of the FAU, Prof. Dr. Harald Bolt, Board Member of Forschungszentrum Jülich, Prof. Dr. Achim Bachem, Chairman of the Board of Forschungszentrum Jülich and Thomas Frederking, Administrative Director of HZB.

Research foci at HI ERN are solutions for printable photovoltaic applications and innovative methods for the chemical storage of solar energy using hydrogen. Another focus is system technologies relating to hydrogen. HZB is contributing its internationally recognized expertise in thin-film photovoltaics and solar-produced hydrogen, a topic currently undergoing significant expansion at HZB. “We want to make the thin-film technologies so far used for producing novel solar cells also usable for solar fuel production. HZB has unique know-how in this field,” says Prof. Anke Kaysser-Pyzalla, scientific director of HZB. Among other things, HZB will be funding a W2 professorship in this field, and will grant the scientists from Nuremberg and Erlangen access to the unique infrastructures at HZB. “Our involvement in HI ERN is also a message that HZB is aligning itself more strongly as a modern energy research centre with a focus on materials research,” Anke Kaysser-Pyzalla stresses.

arö

NEW SPECIAL RESEARCH FIELD: METAL OXIDE/WATER SYSTEMS

Metal oxides enhance special glasses, improve ceramic medical implants and are hot candidates for applications in fuel cells, solar cells, microelectronics and novel catalysts. Accordingly, as of 2013 and until 2017, the German Research Foundation is funding the special research field “molecular insights into metal oxide/water systems”, in which HZB researchers are involved. Dr. Bernd Winter of the junior group led by Prof. Dr. Emad Aziz is studying metal ions and metal oxide complexes in aqueous solution using photoelectron spectroscopy at BESSY II. These measurements yield information on the interactions between the metal oxide complexes and the surrounding water molecules. They can also detect precursor molecules that precede the formation of larger metal oxide networks. These findings are important for synthesising metal oxides in a targeted manner for specific applications. Spokesman for the special research field is Prof. Dr. Christian Limberg of Humboldt-Universität zu Berlin. Other partners are Freie Universität Berlin, Technische Universität Berlin, the University of Potsdam, the Federal Institute for Materials Research and Testing and the Fritz Haber Institute.

Dr. Bernd Winter in the experimental hall of BESSY II.

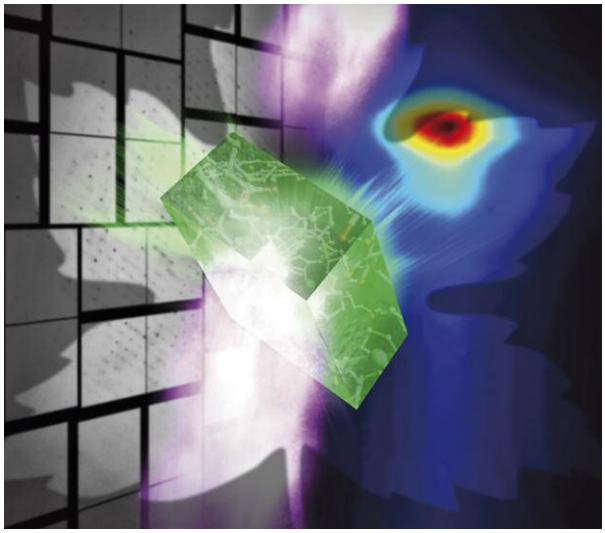
SNAPSHOTS OF PHOTOSYNTHESIS IN ACTION

A German–American team will be making ultrafast snapshots at a modern photon source to observe the intermediate steps in the **complex catalytic reaction of photosynthesis**, a core process of life.

Although all animal organisms consume oxygen, we are thankfully not running out of oxygen just yet. Our thanks go to the green plants, algae and cyanobacteria, which namely use carbon dioxide, water and sunlight to build new molecules through photosynthesis and release oxygen in the process. The core reaction in the "photosystem II" protein, namely the splitting of oxygen from water, is made possible by a catalyst – a complex molecule with a core of Mn_4CaO_5.

What exactly goes on in the reactions involving this natural catalyst is the topic of study of a group involving HZB physicist Dr. Philippe Wernet, chemist Prof. Dr. Athina Zouni of Humboldt-Universität zu Berlin, Dr. Uwe Bergmann of the SLAC National Accelerator Laboratory and Dr. Junko Yano of the Lawrence Berkeley National Laboratory, who is leading the project. Their approach goes far beyond conventional low-temperature X-ray crystallography and X-ray spectroscopy: The intense, ultrashort femtosecond X-ray pulses at the Linac Coherent Light Source, a free-electron laser at the SLAC National Accelerator Laboratory in Stanford, allow them to collect data at room temperature, capturing the signal before the sample is destroyed. "We take a kind of snapshot of the reaction," explains Philippe Wernet.

The researchers are using this method to study the protein structure and the dynamics of the reaction at the Mn_4CaO_5 cluster while light is still being absorbed and water is being oxidized to oxygen. "We are planning a series of time-resolved X-ray scattering and X-ray spectroscopic experiments in order to study the reaction at room temperature and depict all intermediate steps involved," Wernet explains. They hope to gain a highly detailed insight into the reactions that are required for the process of photosynthetic water oxidation. The Human Frontier Science Program has secured funding for this of 900,000 US dollars for the next three years. *arö*



The German-American team is studying core reactions of photosynthesis at light sources such as SLAC and BESSY II.

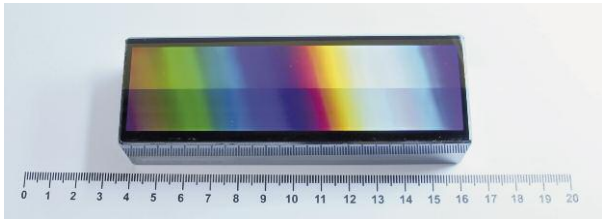
THIN-FILM SOLAR CELLS MADE OF CRYSTALLINE SILICON

HZB and Masdar PV – a company that develops and produces thin-film solar products and solutions – have been working together since 2013 on developing the next generation of thin-film silicon technology. "Thin-film photovoltaic modules based on crystalline silicon can achieve a high efficiency at relatively low material costs," says Prof. Dr. Bernd Rech, head of the HZB Institute for Silicon Photovoltaics. "The advantages of the established wafer-based, crystalline silicon photovoltaics can be combined with those of thin-film silicon technology. The cooperative partners are looking to achieve an efficiency with the new technology that is comparable to that of wafer-based silicon modules. "We expect thin-film solar cells made of crystalline silicon to achieve an efficiency of 14 percent per cell in the shortterm, and are confident that rapid technological progress in this area is possible," says Prof. Rutger Schlatmann, head of the technology transfer unit PVcomB at HZB. Masdar PV has made it its goal to transfer this technology into its existing production facilities and apply it in modules of up to 5.7 square metres in surface area. *hs*

NEW BLAZED GRATINGS FOR PHOTON SOURCES

The Technological Centre for Optical Precision Gratings at HZB has made a breakthrough in the production of **optical components**. It will soon be able to provide blazed gratings to establishments worldwide.

Gratings are used in photon sources for diffracting the light and for filtering out the wavelength needed for the experiments. After two and a half years' work, the developers have now produced the first blazed gratings of highest precision that fulfil the requirements for scientific experimentation. These blazed gratings (also known as echelette or sawtooth gratings) were successfully tested at the electron storage ring BESSY II. They behaved



Blazed grating produced at HZB.

The sawtooth structures are created in this machine. A diamond rules the tiniest of grooves into the gold-coated silicon substrate.

exactly as researchers had theoretically predicted. The Technological Centre for Optical Precision Gratings, led by Dr. Bernd Loechel, Dr. Friedmar Senf and Prof. Dr. Alexei Erko, is the world's only producer of high-efficiency blazed gratings for use at photon sources. The project is funded by the European Union from the EFRE funds.

A blazed grating consists of a silicon substrate with a very thin layer of gold applied to it by vapour deposition. Tiny grooves are ruled into it with a diamond to create the light-diffracting grating structure. Looked at under the microscope, this structure resembles many tiny little sawteeth. Such a grating has 600 sawteeth per millimetre scored into it. Ambient temperatures must not deviate by any more than 0.02 degrees kelvin during the entire process. To ensure that the grating allows as much light of the respective wavelength through as possible, the sawteeth have to be especially flat. This is achieved by treating the gold layer of the ruled grating in an ion-etching plant to flatten the slope on the sawteeth. The developers at HZB have managed to reduce the angle to just two degrees.
"To create these blazed gratings, we had to pick up a lot of technological processes and learn to master them," says Friedmar Senf, who was involved in the EFRE project at HZB. With no other groups working in this field, they had no fund of experience to fall back on. The former manufacturer, C. ZEISS, stopped producing high-precision gratings in 2008. Since then, no new gratings for photon sources had been produced. With their success, the researchers soon hope to close this gap. "The demand for gratings is very high – and our list of orders is long," says Senf.

Innovative gratings for free-electron lasers

The team at the technology centre only started with the actual developmental work at the beginning of 2013. The two years before that were spent building the laboratory facilities at HZB and overhauling the equipment and machinery taken over from ZEISS. "A lot of time passed before our ruling engine was actually fit for this extremely precise work. Among other things, its entire electronics have been renewed. Which is why we are all the more happy to have succeeded in producing functioning gratings in a relatively short time," Friedmar Senf recounts. The team is also developing other innovative gratings, including so-called toroid gratings on curved substrate surfaces, variable line-density gratings and reflection zone plates for use on free-electron lasers. sz

TECHNOLOGY TRANSFER PRIZE FOR DEVELOPMENT OF OPTIMISED CUTTING TOOLS

Dr. Manuela Klaus and Prof. Dr. Christoph Genzel received the 2013 Technology Transfer Prize of HZB. They developed a **novel analytical method** for the structure-property relationships of complex-shaped, coated cutting tools.

For their work, a collaboration with Walter AG in Tübingen, Manuela Klaus and Christoph Genzel used the synchrotron radiation produced in the electron storage ring BESSY II. From the insights they gained, they managed to successfully patent and launch a product line of cutting tools with outstanding wear properties. They are far superior to the competing products on the market.

Research with a view to societal challenges

On behalf of the jury at the award ceremony in October, Prof. Dr. Ehrenfried Zschech of the Fraunhofer Institute for Applied Microelectronics and Nanotechnology Dresden (IZFP) emphasized the importance of this work: “In cooperation with an industrial partner, the prize winners have brought residual stress analysis for stacked, thin-coated materials to such maturity that they can already be used as standard procedures in a number of companies today. The work of Manuela Klaus and Christoph Genzel is an excellent example of technology transfer at HZB.”
The scientific director of Helmholtz-Zentrum Berlin, Prof. Dr. Anke Kaysser-Pyzalla, stressed that HZB “as a member of the Helmholtz Association is researching into fundamental questions – but always with a view to the societal challenges. With technology transfer, we bring insights from top research into application and make a very tangible contribution towards maintaining welfare in the country. We also offer industrial partners an excellent service with our large facilities BESSY II and BER II – and, not least, educate specialists for the economy.”

Twelve contestants – one winner

The HZB Technology Transfer Prize of 5,000 euros was sponsored by LIMO Lissotschenko Mikrooptik GmbH. Managing Director, Dr. Paul Harten, said at the award ceremony: “Our company is also very active in technology transfer. Among others things, we collaborate very closely with colleagues of Helmholtz-Zentrum Berlin on the advancement of technologies. So we are proud to be able to honour HZB’s achievements in technology transfer with this prize.” An external specialist jury of renowned experts judged the twelve submitted technology transfer projects according to their degree of innovation and market potential. Five candidates presented their concepts during the award ceremony: the presentations impressed the jury, who then announced the winning team. This was the seventh Technology Transfer Prize awarded by HZB for outstanding achievement in the field of technology transfer.

sz/arö

Manuela Klaus presents a "Silver Tiger" cutting tool.

Manuela Klaus and Christoph Genzel developed a way to produce very low-wearing cutting tools. They received the HZB Technology Transfer Prize for this achievement.

EMIL IS TAKING SHAPE

The research building for the new laboratory EMIL at BESSY II came a **long way forward in 2013**: from ground-breaking ceremony to topping-out ceremony in just four months.

In December 2013, the "Energy Materials In-Situ Laboratory Berlin", EMIL, celebrated its topping-out ceremony. "Only four months after the ground-breaking ceremony, EMIL now has a roof over its head," HZB's scientific director Prof. Dr. Anke Kaysser-Pyzalla said at the event. "That makes us confident that we will be commencing research

High-tech building beside high-tech building: The "Energy Materials In-situ Laboratory Berlin" (EMIL) is being built directly adjacent to the synchrotron light source BESSY II of HZB. Those interested can follow the progress of EMIL's construction as captured by an onsite webcam: http://www.helmholtz-berlin.de/projects/emil/webcam/index_de.html

in the new, ultra-modern preparation and analytical laboratory for solar energy and catalysis research on schedule in 2015."

Interdisciplinary and industrial-compatible research

The "Energy Materials In-situ Laboratory Berlin" – EMIL for short – is being built directly onto the synchrotron light source BESSY II of HZB in Adlershof. The joint project of HZB and the Max Planck Society will in future offer a unique infrastructure for the interdisciplinary and industrial-compatible development of novel materials and technologies. These are sorely needed for the success of the energy turnaround. They include new materials systems for solar modules and storage solutions for which novel catalysts must be developed. "Staring from 2015 at EMIL, we will be able to analyse under real conditions – even during the manufacture of thin-film solar cells or catalysts – what processes take place at boundaries and make depth-resolved observations of these," says project head Prof. Dr. Klaus Lips. This will provide a fresh boost for the industrial manufacture of such components, Lips is convinced.

Research for the energy turnaround

In their plan to improve and develop new photovoltaic and catalytic materials, structures and components, the EMIL scientists will be using an infrastructure that is unique in the world. It combines a wide range of the latest preparation technologies from various material classes with dedicated X-ray analytics at the synchrotron BESSY II into one system. "This 'in-situ' approach allows us to study materials, structures and components between successive and, in some cases, even during certain preparation steps along the path towards the finished component," Klaus Lips explains. "That way, we can gain deep insights into the physical and chemical processes governing the component's function."

Furthermore, directly combining different material classes – such as organic and inorganic semiconductors – into novel hybrid structures and components creates synergies and allows the exploration of novel functional mechanisms. Klaus Lips concludes: "Our aim is to determine beyond doubt the structure-function relationship in novel photovoltaic and photocatalytic systems, and thereby play a key role in shaping the future generation of solar energy-converting components."

The construction of EMIL, with its analytical tools SISSY and CAT, is being funded with 18 million euros. HZB is investing 6 million euros in EMIL and the Max Planck Society is participating with a further 6.7 million euros. The German Federal Ministry for Education and Research (BMBF) is funding construction of the SISSY end station with 5.7 million euros from the "Photovoltaics" innovation alliance. "Realizing EMIL together with the Max Planck Society and creating the best analytical conditions for researchers worldwide would have been inconceivable without the fusion of the Hahn-Meitner Institute and BESSY in 2009. The new EMIL project makes the benefits of the merger especially clear," says Prof. Dr. Anke Kaysser-Pyzalla. *hs*

FINISH LINE FOR THE HIGH-FIELD MAGNET

After five years' construction time in the USA, the **superconducting coil** of HZB's new high-field magnet (HFM) was completed in 2013. It was then installed into the cryostats in Italy before arriving at HZB in January 2014.

The arrival of the 6-tonne magnetic coil in Italy marked an important milestone in the construction of the high-field magnet: The superconducting magnetic coil was finally complete. Around 50 people of the National High-Magnetic-Field Laboratory in Tallahassee (NHMFL), USA, carried out this developmental work together with the 8-head-strong HFM project team of Helmholtz-Zentrum Berlin. More than 96,000 NHMFL man-hours went into the development and construction of the superconducting coil. Before the magnet left the States, this achievement was celebrated at a ceremonial handover at the National High-Magnetic-Field Laboratory in Tallahassee. Attending the ceremony were the project head, Dr. Peter Smeibidl, and then director of the Hahn-Meitner Institute, Prof. Dr. Michael Steiner. Scientific director of HZB, Prof. Dr. Anke Kaysser-Pyzalla, conveyed a personal message by telephone during the ceremony.

A milestone is reached after five years of developmental work: This is what the new superconductive coil of the new high-field magnet looks like.

Up to 26-tesla field strength

In Chivasso, Italy, the experts from the company Criotec manufactured the cryostats that will keep the magnet cool, and built the coil into them. At the end of January 2014, the preassembled magnet then arrived at Helmholtz-Zentrum Berlin, where its final installation commenced. This included installation of the normally conducting, resistive coil. Once testing of the magnet's full functionality is complete, it will be connected to the neutron guide, probably in the autumn of 2014. By then, the scientists working with Dr. Peter Smeibidl will have built the necessary infrastructure for current and cold supply and carried out extensive performance tests.

The HFM will achieve a field strength of around 26 teslas, making it the strongest magnetic field for neutron scattering. So far, only magnetic fields of up to 17 teslas have been combined with neutron scattering. Researchers expect their neutron experiments – under strong magnetic fields and low temperatures – to yield especially enlightening insights into the behaviour of materials, including semiconductors. Since September 2013, project management for completion of the high-field magnet and neutron instrument EXED has been in the hands of Dr. Peter Smeibidl.

SZ

MAGNETISM IN BASIC RESEARCH

At the neutron instrument EXED, HZB's new high-field magnet will generate magnetic fields of more than 25 teslas. Magnetism plays a crucial role in basic and materials research for understanding the properties and behaviour of different materials. Experiments using neutrons are especially suitable for studying these magnetic material structures. With the unique experimental opportunities under extremely high magnetic fields, researchers hope to discover new phenomena and gain a better understanding of promising materials.

HZB LAUNCHES ITS FIRST GRADUATE SCHOOL

MATSEC, HZB'S VERY OWN **GRADUATE SCHOOL**, WAS LAUNCHED IN OCTOBER 2013.

The graduate school is located at the Dahlem Research School (DRS) of the Freie Universität Berlin (FU Berlin). A total of ten HZB doctoral students can take advantage of the MatSEC in parallel to working on their doctorates. The graduate school has its focus in the research of kesterites, novel material systems for photovoltaics. Professor Dr. Susan Schorr, HZB department head for crystallography and professor at the FU Berlin, is the speaker for the new graduate school. Involved as partners are workgroups of the FU, TU and HU Berlin as well as the TU Cottbus.

Prof. Dr. Susan Schorr (first row, middle), speaker of the graduate school "Materials for Solar Energy Conversion" (MatSEC) at HZB, amongst the staff and the first doctoral students.

YOUNG INVESTIGATOR PRIZE FOR KATHRIN AZIZ-LANGE

The Wilhelm-Ostwald Prize for Young Investigators was awarded to Dr. Kathrin Aziz-Lange in March 2013 for her doctoral thesis prepared at HZB. The award includes prize money of 2,500 euros. Prepared while working with Professor Emad Aziz' young investigator group, Kathrin Aziz-Lange's doctoral thesis made a decisive contribution towards enriching the experimental techniques for liquid spectroscopy with photon beams. She developed methods which made it possible to investigate chemical and biological samples – for example, proteins – in their natural environment. Among other things, she made important findings about hydrogen bonds in liquids and about the thermodynamic behaviour of ions in solution.

HUMBOLDT RESEARCH PRIZE FOR STEPHEN CRAMER

Professor Stephen P. Cramer, renowned expert for synchrotron spectroscopy, was awarded a Humboldt research prize in December 2013 endowed with prize money of 60,000 euros. This will allow him to work in close cooperation with a team at the Helmholtz Centre Berlin and the Freie Universität Berlin during 2014. Cramer is professor for advanced light sources at the University of California, Davis, and researches at the Lawrence Berkeley National Laboratory.

25 YEARS OF OUR SUMMER STUDENT PROGRAMME

A total of 24 students from 13 countries used their semester break in September 2013 to pursue their own projects at the Helmholtz Centre and to gather their first experience in research. With the international summer student programme, HZB has been offering young adults from all over the world insights into the world of energy and materials science since 25 years. The physics, chemistry or engineering students are looked after during the eight-week period by experienced researchers.

ORGANISATIONAL CHANGES AT HZB

SEVERAL **FUNCTIONS** AND **POSITIONS** WERE REORGANISED IN THE HELMHOLTZ CENTRE BERLIN DURING 2013.

Professor Dr. Bernd Rech became the energy division speaker in 2013, with Professor Dr. Rutger Schlatmann appointed his deputy. Professor Dr. Bella Lake was appointed speaker for the M division, with Professor Dr. Susan Schorr her deputy. Dr. Klaus Habicht succeeds Professor Dr. Alan Tennant, and automatically becomes a new member in the steering committee of the user platform for the neutron division. Acting head of the institute "Complex magnetic materials" is Professor Dr. Susan Schorr, whereas the department "Magnetisation dynamics" is being temporarily headed up by Professor Dr. Oliver Rader. The department "Researching with spallation neutrons" has been renamed "Methods for the characterisation of transport phenomena in energy materials" (G-AMCT for short). Dr. Klaus Habicht is the director. Dr. Stephan Welzel was appointed deputy head of the reactor department. Dr. Karin Haas, who held this position before, now heads up the reactor safety department. There is now a new department in facility management called "Planning and building" which is headed by Frank Uschkoreit.

PROFESSOR DR. ALAN TENNANT LEAVES HZB

Professor Dr. Alan Tennant was appointed chief scientist at the Neutron Sciences Directorate of the Oak Ridge National Laboratory (ORNL), and left the Helmholtz Centre Berlin in November 2013. Tennant came to Berlin in 2004 and his last post here was speaker of the magnetism division. In addition, he headed the Institute for Complex Magnetic Materials and the department for magnetisation dynamics. After being able to prove the existence of magnetic monopoles at the Berlin research reactor BER II in 2009, his team received international acclaim – the trade magazine Science numbered this work among the top 10 breakthroughs of 2009.

DR. TRISTAN PETIT JOINS THE AZIZ TEAM

In the summer of 2013, Dr. Tristan Petit joined Professor Dr. Emad Flear Aziz' team for two years as a postdoctoral researcher in order to continue his research into nanodiamonds and their biomedical potential. His Humboldt Foundation Fellowship for Postdoctoral Researchers permitted Petit to select his own scientific host in Germany, and he decided on the Joint Ultrafast Dynamics Lab in Solutions and at Interfaces (JULiq) that was set up by Aziz.

IMPORTANT APPOINTMENTS

Prof. Dr. Martina Schmid, head of the Helmholtz young investigator group "Nanooptical concepts for photovoltaics" (NanooptiX) at HZB since November 2012, was appointed junior professor at the Freie Universität Berlin (FU). Besides her research at HZB, she now also teaches at the FU department of physics.

Prof. Dr. Silke Christiansen was appointed a W3 professor for the physics department of the Freie Universität Berlin (FU) in November 2013. Since January 2013, Silke Christiansen has been heading the newly established institute "Nanoarchitectures for Energy Conversion" at HZB, and is considered an internationally recognised expert on nanostructures for thin-film solar cells.

Organisation Chart HZB

Date March 2014, Rev. 03. March 2014 GB

HZB Helmholtz Zentrum Berlin

General Meeting of Shareholders (German Federation and State of Berlin)

Supervisory Board (Vorsitzender: Prof. Dr. J. Treusch)

Scientific Advisory Council Chairwoman: Dr. U. Steigenberger

Science and Technology Board Vorsitzender: Prof. Dr. R. van de Krol

Works Council Chairwoman: E. Lesner

Geschäftsführung

Wissenschaftliche GF Prof. Dr. A. Kaysser-Pyzalla

Kaufmännische GF Th. Fredeking

Communication (Dr. I. Helms)

Directors´ Office (Dr. B. Meißner)

Safety

Compliance Management (C. Pursian)

Solar Energy Research
Speaker: Prof. Dr. B. Rech E

- **Silicon Photovoltaics** (Prof. Dr. B. Rech) E-IS
- **Heterogeneous Materials Systems** (Prof. Dr. M. Lux-Steiner) E-IH
- **Solar Fuels** (Prof. Dr. R. van de Krol) E-IF
- **Competence Centre Photovoltaics Berlin (PVcomB))** (Prof. Dr. R. Schlatmann) E-IP
- **Nano-architectures for Energy Conversion** (PD. Dr. S. Christiansen) E-IN
- **Nanospectroscopy for Energy Material Design and Optimization** (Dr. S. Raoux) E-ISPEK
- **Complex Compound Semiconductor Materials for Photovoltaics** (Dr. Th. Unold*) E-AKV
- **Interface Design** (Prof. Dr. M. Bär) E-NI
- **Nanooptical Concepts for PV** (Prof. Dr. M. Schmid) E-NOPT
- **Nano-SIPPE** (Dr. C. Becker) E-NSIP
- **Molecular Systems** (Prof. Dr. N. Koch) E-GMS
- **Catalysis for Energy** (Prof. R. Schlögl) E-GKAT

Large Scale Facilities
Speaker: Prof. Dr. A. Föhlisch G

- **Methods and Instrumentation for Synchrotron Radiation Research** (Prof. Dr. A. Föhlisch) G-ISRR
- **Accelerator Physics** (Prof. Dr. A. Jankowiak) G-IA
- **SRF – Science and Technology** (Prof. Dr. J. Knobloch) G-ISRF
- **Nanometre Optics and Technology** (Prof. Dr. A. Erko*) G-INT
- **Methods for Characterization of Transport Phenomena in Energy Materials** (Dr. K. Habicht) G-AMCT
- **Undulators** (Dr. J. Bahrdt) G-AUND
- **Simulations of ERL-Designs** (Prof. Dr. A. Matveenko) G-NSIMU
- **Neutron Tomography** (Prof. Dr. W. Treimer) G-GTOMO

Magnetic Materials
Speaker: Prof. Dr. B. Lake M

- **Magnetisation Dynamics** (Prof. Dr. O. Rader*) M-AMD
- **Quantum Phenomena in Novel Materials** (Prof. Dr. B. Lake) M-AQM
- **Crystallography** (Prof. Dr. S. Schorr) M-AKR
- **High Field Magnet** (Prof. Dr. B. Lake*) M-AHFM

Functional Materials
Speaker: Prof. Dr. M. Ballauff F

- **Applied Materials** (Prof. Dr. J. Banhart) F-IAM
- **Soft Matter and Functional Materials** (Prof. Dr. M. Ballauff) F-ISFM
- **Microstructure and residual stress analysis** (Prof. Dr. Ch. Genzel) F-AME
- **Functional Materials in Solution** (Prof. Dr. E. F. Aziz Bekhit) F-NFF
- **Functional Nanomaterials** (Prof. Dr. S. Eisebitt) F-GFN
- **Ultrafast Dynamics** (Prof. Dr. M. Bargheer) F-GUD

User Platform
Speaker: Prof. Dr. A. Jankowiak NP

- **User Coordination** (Dr. Th. Gutberlet) NP-ACO
- **Operation Reactor BER II** (Dr. H. Krohn) NP-ABR
- **Operation Accelerator BESSY II** (Prof. Dr. A. Jankowiak) NP-ABS
  - **MLS Operation** (K. Bürkmann-Gehrlein) S-MLS
- **Protons for Therapy** (Dr. A. Denker) S-PT
- **Precision Gratings** (Dr. M. Lörgen) S-PG
- **Scientific-Technical Infrastructure 1** (Dr. A. Rupp) NP-HI
  - **Technical User Support BER II** (Dr. A. Rupp) NP-AUN
  - **Sample Environments** (Dr. K. Kiefer) NP-ASE
  - **Technical Design** (L. Drescher) NP-ATD
  - **Manufacturing** (K. Tietz) NP-AMAN
- **Scientific-Technical Infrastructure 2** (Dr. C.Jung) NP-HII
  - **Technical User Support BESSY II** (Dr. C. Jung) NP-AUP
  - **Experiment Control and Data Acquisition** (O. -P. Sauer) NP-AED
  - **Networks & Storage** (Dr. D.Herrendörfer) NP-ASN

Administration
(U. Ewald) A

- **Personnel and Social Matters** (M. Badel) A-PS
- **Finances and Accounting** (J. Neumann) A-FR
- **Purchasing and Materials Logistics** (D. Höcker) A-EM
- **Third Party Funding** (Dr. Y. Tomm) A-DM

Facility Management
(Dr. B. Schröder-Smeibidl) FM

- **Planning and Construction** (F. Uschkoreit) FM-B
- **Technical Services** (U. Grabe) FM-T
- **Central Data Processing and Networks** (I. Heinzel*) FM-D
- **Internal Services** (M. Nadolski) FM-I
- **Chemicals and Special Wastes** (J. Beckmann) FM-C
- **Berlin Collection Point of Radioactive Waste** (J. Beckmann) S-ZRA

Institute | Young Investigator Group | Special Task

Working Group | Joint Research Group | Committee

* Acting Head

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

IMPRINT

HZB Highlight Report 2013 of the Helmholtz-Zentrum Berlin für Materialien und Energie GmbH. Reprint only with the express permission of the publisher.
Press date: July 2014

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

Editors:
Dr. Ina Helms (ih, responsible), Hannes Schlender (hs, coordination), Antonia Rötger (arö), Silvia Zerbe (sz)
E-mail: ina.helms@helmholtz-berlin.de, address as for publisher

Publishing services & support:
n.k mediaconcept GbR, Obere Lagerstraße 38b,
82178 Puchheim bei München, Tel.: +49 (0)89 80 90 83 33
Managing directors: Klaus Dieter Krön, Christoph Neuschäffer

Concept & realisation:
Christoph Neuschäffer (cn), Tel.: +49 (0)89 20 20 68 66

Editorial staff: Ralf Butscher (rb), Roland Knauer (rk), Torsten Mertz (tm), Heidi Tiefenthaler (ht)

Translation: Peter Gregg, Gill Elaine Schneider

Design & layout: Klaus Dieter Krön

Picture editor: Christoph Neuschäffer

Picture editing: Lothar Trutter

Proofs: Trumedia Gmbh, Tattenbachstraße 19, 86179 Augsburg

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

Photo credits: all photo rights remain with HZB, except for: page 2/3 HZB/Barbara Baier, page 8 HZB/Michael Fernahl, page 11 BMW AG, page 12 Uni Duisburg-Essen, page 14 Gerald Eisenblätter, page 15 Malte Behrens, page 16 Yazdani Lab, Princeton University, page 18 C. Steegborn, page 19 University of Oulu, page 20 NanoTechCenter Weiz, page 23 Tennen-Gas/wikipedia.de, page 24 André Bisig, Johannes Gutenberg Universität Mainz, page 25 RUB, modified from Physical Review Letters, page 26 HZB/Pia Fernahl page 31 Hirohito Ogasawara, SLAC National Accelerator Laboratory, page 33 Georg Heimel/HU Berlin, page 34 Didier Descouens/wikipedia.de, page 36 Greg Stewart, SLAC National Accelerator Laboratory, page 38 R. Mainz/A. Singh, page 42 HZB/Frieder Müller, page 43 TU Delft, page 45 H. D. Wöhrle/Universität Göttingen, page 46 Stephan Thürmer, page 47 Greg Stewart, SLAC National Accelerator Laboratory

Contacts

Lise-Meitner-Campus

Hahn-Meitner-Platz 1
14109 Berlin
Germany
Tel.: +49 (0)30 8062 - 0
Fax: +49 (0)30 8062 - 42181
wannsee@helmholtz-berlin.de

Wilhelm-Conrad-Röntgen-Campus

Albert-Einstein-Str. 15
12489 Berlin
Germany
Tel.: +49 (0)30 8062 - 0
Fax: +49 (0)30 8062 - 12990
adlershof@helmholtz-berlin.de

Silicon photovoltaics

Kekuléstr. 5
12489 Berlin
Germany
Tel.: +49 (0)30 8062 - 0
Fax: +49 (0)30 8062 – 41333
E-IS-office@helmholtz-berlin.de

PVcomB

Schwarzschildstr. 3
12489 Berlin
Germany
Tel.: +49 (0)30 8062 - 0
Fax: +49 (0)30 8062 - 15677
info@helmholtz-berlin.de