HZB Helmholtz Zentrum Berlin

ENERGY IS OUR MATTER

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HIGHLIGHTS 2019/2020

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

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FOREWORD

Two extremely intense years lie behind us. We shut down the BER II neutron source at the end of 2019 as planned, and the Helmholtz-wide institutional evaluations were barely completed when the corona pandemic hit us at HZB as well. We have had to severely restrict user operations at BESSY II since March 2020. Laboratory operations were also shut down, and many employees organised and performed their work remotely. Nevertheless, amazing research results have again been achieved at the HZB in 2019 and 2020. We would like to present a selection of them to you in this two-year report on the highlights.

Neutron experiments from BER II are being presented in this issue for the last time. For almost five decades, BER II has facilitated deep insights into the structure of materials. We had long prepared for the scheduled shutdown in December 2019. This advanced planning made it possible to arrange the transfer of the specialised BER II experimental equipment to other neutron sources for continued use. Read more about this on page 40.

Thomas Frederking, © HZB/M. Setzpfandt

In all of our research fields – energy, information, and matter – the scientific productivity and international profile of HZB has remained high, despite the coronavirus. Great attention was attracted, for example, by the two world records that HZB teams set for two different tandem solar cells. In addition, we were able to initiate a new catalysis centre together with the Max Planck Society as a beacon project named CatLab. Learn more about it on page 5.

During the lockdown and remote-work period, we promoted and constantly improved scientific exchange by means of new digital platforms. Even the User Meeting at the end of 2020 had to take place digitally and was a great success, with 460 participants. We gained experience that we can also build on in the future, including close collaboration via digital modes and conducting experiments remotely. Our ecology team believes this could be good news for the environment because air travel has thus far accounted for a significant proportion of the HZB's greenhouse gas emissions. Nevertheless, we very much hope that we will soon be able to welcome scientists from the world over to conduct their experiments with us again.

Thomas Frederking
Commercial Director

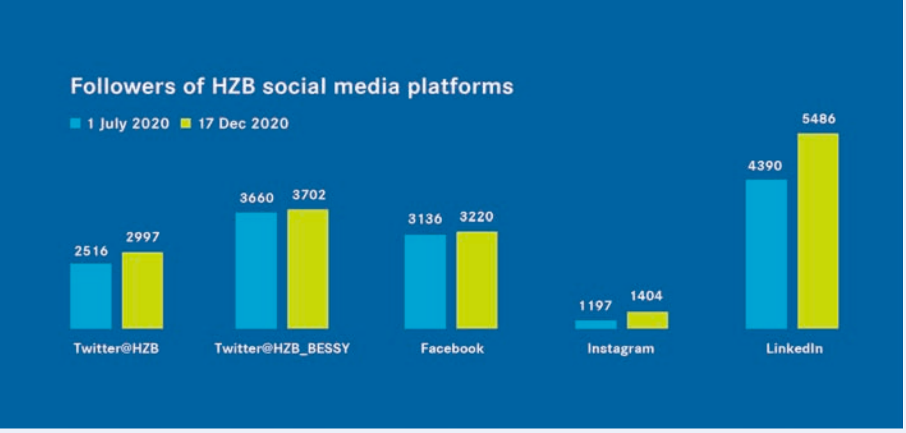
Bernd Rech
Scientific Director

Jan Lüning
Scientific Director

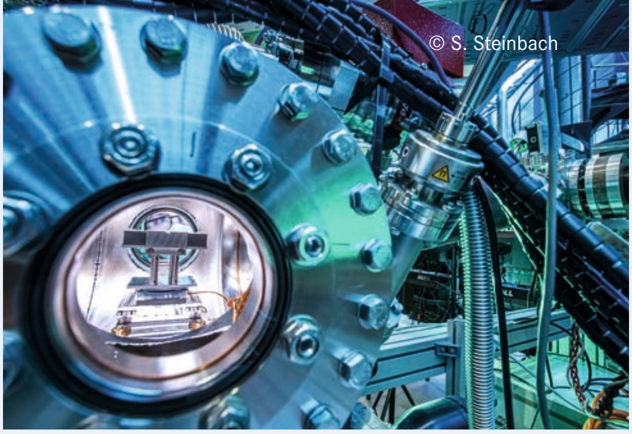
STAY UP TO DATE WITH THE HZB NEWSLETTER

Would you like to receive regular news from the HZB? We would be happy to send you the monthly newsletter (in German). You can subscribe here: **hz-b.de/newsletter**

The BESSY newsletter is oriented primarily towards the international user community of BESSY II. It provides information in English about developments at BESSY II. You can subscribe here: **hz-b.de/newsletter-en**



Blog & YouTube visits Jan. 2019 - Dec. 2020:
Campusblog: 110,000; Scienceblog: 80,000;
YouTube videos: 50,000



All around the HZB: hz-b.de/virtuelle-rundgaenge
Tour of the BESSY II accelerator and more:
hz-b.de/insights-bessy2

DESPITE THE PANDEMIC: HZB CONNECTS TO THE PUBLIC

Communication and exchange with society is important to the HZB. We welcome visitor groups, offer project days in the School Lab, participate in the Long Night of the Sciences and organise events such as Physics for Breakfast and Open House Days. We had to continue all of these as digital events in 2020. Nevertheless, the HZB remained in the public eye during the year of the corona pandemic.

96
visitor groups in 2019 viewed the BESSY II synchrotron, the BER II research reactor, the research laboratories, and spoke with HZB researchers – a total of more than 1,800 people.

about **2,500**
YouTube clicks were registered by the BESSY II video tour during the 2020 Long Night of the Sciences.

4,400
internet viewers via Radio TEDDY. The HZB presented an experiment each week for 12 weeks in 2020 as a media partner. The experiments were presented as videos on the editorial website of the radio station.

150
people accessed the online presentations of the HZB during Berlin Science Week in November 2020. This was provided as a live stream offering viewers their choice of a panel discussion on the topic of photovoltaics, a lecture on drug development aided by protein structure analyses, and a virtual tour through BESSY II.

1,300
visitors enjoyed the Long Night of the Sciences at HZB Wannsee in 2019. 475 people took guided tours of BER II.

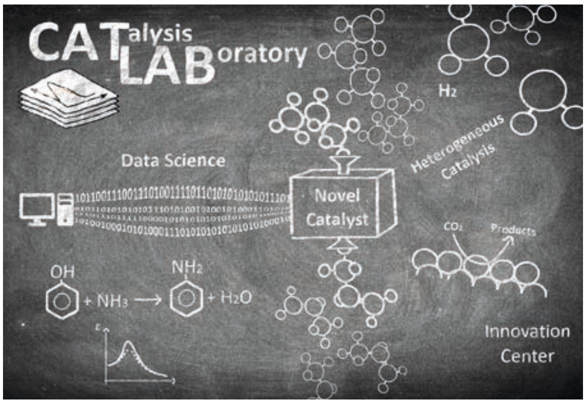
127
News and Science Highlights were published in 2020 and accessed 400,000 times.

approx. **1,300**
people received the HZB monthly newsletter in 2020. The BESSY II newsletter (English) reached more than 300 people per month.

CatLab – a beacon for hydrogen research

Catalysts are key for the many technologies and processes required to make the **economy climate-neutral**. **Innovative catalytic processes** are needed to produce hydrogen and synthetic fuels using renewable energy. The German federal government's National Hydrogen Strategy clearly identifies research as the basis for leaps in innovation. The HZB is now setting up a research infrastructure in Berlin named CatLab with partners from the Max Planck Society.

The Helmholtz-Zentrum Berlin (HZB) is working on this with the Fritz Haber Institute (FHI) and the Max Planck Institute for Chemical Energy Conversion (MPI CEC). "We are establishing the CatLab infrastructure in the immediate vicinity of the BESSY II synchrotron radiation source in Berlin-Adlershof in order to achieve synergistic research focussed on catalysis. There,



© HZB/S. Hlawenka

the most modern synthesis and analysis methods are available to analyse chemical and physical processes during the catalytic reactions at the atomic level of resolution and in real-time", says Bernd Rech, Scientific Director at the HZB. Robert Schlögl, Director at the FHI and MPI CEC emphasises: "We have already set up over the last few years a unique *operando* measurement infrastructure at BESSY II that will complement CatLab perfectly. We were able to use this to create a new functional model of catalysts optimised by means of thin-film technology. Now we are going to conduct these activities under the umbrella of CatLab to expand and advance them."

The chemical industry is also involved. BASF is participating in the setup and scaling of the processes and development of the reactors. In addition, there are collaborations with Humboldt Universität, the UniSysCat Cluster of Excellence and the BasCat Laboratory (TU Berlin and BASF). Additional partners can be integrated via these collaborations.

German Federal Minister of Education and Research Anja Karliczek wishes the project every success and emphasises: "Sustainably produced hydrogen is an opportunity of the century for a highly industrialised country like Germany, and for climate protection worldwide. In order to make sustainable hydrogen an economic success, we need to make leaps in innovation. CatLab is superbly positioned to do this. Through collaboration between the MPG and HZB that is embedded in Berlin's research landscape, and with participation from private industy, CatLab focusses cutting-edge expertise along the entire innovation chain."

Infrastructure for catalysis research is being created in Berlin in order to achieve innovative leaps in hydrogen research. For this purpose, the **Helmholtz-Zentrum Berlin** and **two Max Planck Institutes** are pooling their expertise to jointly establish the CatLab research laboratory together with **Humboldt-Universität zu Berlin**. CatLab is intended to bridge the gap between basic research and industry, and has been funded by the German Federal Ministry of Education and Research with more than 50 million euros. In total, the establishment of the project over five years comprises around 100 million euros.

OUR ENERGY RESEARCH BENEFITS FROM BESSY II

The current funding period of the Helmholtz Association based on the scientific assessment of the Helmholtz Centres during 2017-2018 and on the strategic evaluation of the research topics during 2019-2020 commenced in January 2021. In this interview, **Bernd Rech**, spokesperson for the HZB scientific management, explains what awaits us in the coming years.

HZB has now entered the POF IV programme-oriented funding period. Are you happy with it?
Yes, I am very happy! We've had a great assessment that has given us impetus to continue our cutting-edge research. Our employees are primarily responsible for this. It was a great team effort! I am incredibly curious about the exciting results that will come from research during the next few years.

What opportunities does POF IV hold for the HZB?
We conduct research that is highly relevant for society. We presented our enhanced expertise and ideas in the assessments, including in the fields of solar energy conversion, quantum materials, artificial photosynthesis, and also on the topic of hydrogen. We received above-average ratings for these – as well as for our large-scale facility BESSY II and our work in accelerator physics that is very important for this. As a result of the positive review, we now have been given the green light to implement these ideas and achieve a great deal.

Prof Bernd Rech © HZB/M. Setzpfandt

> "POF IV facilitates long-term planning and provides the financial assurance."

What is the financial impact of POF IV?
The evaluation provides us with a funding increase of two per cent annually – this allows us to plan in a predictable way, but not to make any big leaps. The POF IV funding envelope was established for seven years, which means a long period of financial stability – an excellent situation for us.

The HZB will be involved for the first time in the Helmholtz Research Field of Information. What was the motivation for this?
The Helmholtz-wide Research Field of Information is new. In the many discussions with other Centres of the of the Helmholtz Association, we noticed that our research on quantum and functional materials fits in perfectly here. Up to now, this research has been carried out in the Helmholtz Research Field of Energy. With this administrative step, we can also contribute a great deal in terms of content with our research. Thanks to the proximity to BESSY II and BER II, we have published many exciting results on quantum materials in past years. Even though we are only a smaller partner in the Research Field of Information, we can contribute our particular strengths – the tight integration with BESSY II and our proximity to Berlin's universities.

How do you link research even more closely with the advanced developments at BESSY II?
BESSY II is an inherent part of our research. Our scientists set up new instrumentation and advise users – so are therefore very close to important advances. BESSY II and energy research are not two independent pillars of the HZB, they are a single common one. Energy research benefits from access to BESSY II and BESSY II benefits from the fact that new

questions in science require new research methods. This close connection with energy research is not found at any other synchrotron facility and is our particular strength.

Time has passed between the scientific assessments and the start of POF IV. In the meantime, have you been able to implement a few of the recommendations of the experts?
Of course! We have not put off implementing the recommendations. One of them was, for example, that we needed to boost our activities in catalysis. Catalysis is an ideal fit both to our energy research and to BESSY II. We are currently setting up a new joint beacon project with the Max Planck Society – the CatLab project. Another example: the reviewers in their assessment recommended pushing ahead with tandem solar-cell technology, where we are at the worldwide forefront and which has huge market potential. Here, too, we have invested – and were able to extend our leading position in perovskite tandem solar cells.

The German federal government recently brought in its Hydrogen Strategy. What potential do you see for the HZB?
Substantial. A central question of the strategy is how hydrogen will be produced in an environmentally friendly manner. To contribute to this transition, the hydrogen must be sustainably produced with the help of renewable energies. That is precisely our field of research! We have strengths at both our campuses in artificial photosynthesis, solar fuels, and we are exploring how to convert CO_2 into valuable industrial feedstock. The keyword for this research is catalysis. We must understand the chemical and electronic processes in order to develop new catalysis materials and the associated process and reaction engineering for it that is inexpensive and efficient. With our expertise in thin-film technologies and BESSY II, we can contribute important building blocks that the implementation of the Hydrogen Strategy depends upon.

CatLab, as previously mentioned, is certainly paying off.
Exactly, it is a truly visionary project! It is based on close collaboration with research groups of the Max Planck Society, as well as with industrial participants and the Berlin universities. We are certain that we can accomplish a great deal thanks to our joint and closely-coupled range of expertise. We are able to set up new things and thus create new catalysis technologies to achieve a rapid breakthrough – also thanks in part to the proximity to BESSY II. The CatLab only really makes sense because of the rapid access to synchrotron light.

“BESSY II and energy research are not two independent pillars of the HZB, they are a single common one.”

What role will knowledge transfer play in the future?
Knowledge transfer is a matter close to my heart. We live in a knowledge-based society in which research plays a significant role. Our task is to arouse enthusiasm, but also a comprehension of science, be it with our school laboratory, lectures for children, or during the Long Night of the Sciences event. Augmentation of our perspective is important, because it means we gain new motivation. Our newly founded Consulting office for building-integrated Photovoltaics is very active: it advises urban planners, architects, and builders, and has met with a lot of interest. Knowledge transfer must necessarily be a part of our activities.

POF IV runs until the end of 2027 - that still sounds like a long ways off. Nevertheless, let's look into the future. What technologies will the HZB have set in motion by then?
Okay, so then a look into the crystal ball: new photovoltaic technologies will have made the leap into the marketplace. Some of these would not have got this far without HZB research. Likewise, there are efficient catalysis materials and novel batteries. Ecological hydrogen is no longer a pipe dream, but has become a reality. And our research on quantum materials, which is strong at both campuses, will have identified candidates for efficient information processing. At BESSY II, novel experiments will be underway on state-of-the-art beamlines, supported by artificial intelligence, the user community will have continued to grow, and BESSY III will be well on the way. We will have seen the fruits of our labour arrive to industry and society through our technology transfer programme. But the most important thing is that HZB will be and remain a lively, innovative place to work where talents from the world over come together. We want to continue using our imagination, do exciting research, and achieve breakthroughs in the coming years.

The interview was conducted by Silvia Zerbe and Ina Helms.

IDENTIFYING THE FUTURE NEEDS OF THE COMMUNITY

Jan Lüning was officially appointed Scientific Director of the HZB on June 1, 2019. In this interview, he talks about his initial time at HZB as well as the major tasks involved in upgrading the BESSY II synchrotron radiation source and planning the successor synchrotron source, BESSY III.

The BER II research reactor was shut down at the end of 2019. You only experienced the successful neutron era at the HZB briefly. What has impressed you during this time? And what happens now with the system and the instruments?
The reactor team allowed the users to conduct experiments until the very end. I was in the Experiment Hall as the control rods were gradually pushed in and the neutron flux slowly decreased. Colleagues conducting experiments nevertheless continued to take data, really down to the last neutron. That was a moving moment, certainly somewhat melancholy, but the commitment and enthusiasm for experimentation were clearly evident. The second aspect is the excellent instrumentation that was built at BER II over the years. Our instruments are recognised worldwide for their quality, which is why there is also demand to use them at other sources. As someone who has been involved in the development of instruments, I am especially pleased about that. Meanwhile, new homes have already been found or there are concrete prospects of further use for all the highly specialised instruments used at BER II.

> “We are always in competing with other light sources. So we have to pick up on ideas and recognise what the community will need and want in the future.”

The HZB reviews in January 2018 have highlighted the preeminent importance of BESSY II, especially for energy research. This necessitates maintaining BESSY II at this top level over the next ten years. What measures are planned for this?
After its 20 years of operation, we are planning a fundamental upgrade of BESSY II. All components are included in the medium-term financial planning for the next ten years – from the accelerators, mirrors, and control elements for monochromators to IT elements that support the infrastructure, for example, in order to be able to handle the rapidly increasing volume of data streams produced during the experiments. This implementation has already begun.

This kind of upgrading is typically necessary and expected. What about the larger decision space? What beacon projects could you foresee within the next ten years?
I have to backtrack a little, because the question involves how we dovetail the BESSY II upgrade with our planned successor source, BESSY III. The discussion of the goals for BESSY III simultaneously leads us to consider which ones we might accomplish sooner with the BESSY II upgrade. BESSY II must remain a sought-after source when we submit the application for the construction of the successor in a few years’ time.

That involves the instrumentation. Is there already investment in future instrumentation?
Yes, because we are fighting for the most highly regarded user groups – those found within the HZB as well as external groups! We are always in competition with other light sources. So we have to pick up on ideas and recognise what the synchrotron community will need and want in the future. In doing, so we concentrate on the research fields in which BESSY II can make truly important contributions. We ask ourselves what modes of operation and experiments do we have that no other source offers, and can be adapted to meet a need that no other synchrotron covers.

From the workshops with expert groups that we conducted as part of the BESSY III project, we have already been able to conclude what the core research topics are. We learned what the leading minds need and where they want to go with their research.

What are the most important findings then?
Spatial resolution as well as *in situ* and operando techniques are recurring keywords. In addition, the

Jan Lüning © HZB/HG Medien

heterogeneity of materials is increasingly mentioned. We are moving further and further away from homogeneous, static materials like single crystals. We must offer empirical techniques for studying heterogeneous materials and their particular properties. This plays a major role in quantum materials, for example.

Battery materials are also an important field. There is an enormous amount of research going on in this area, but there is still no dedicated facility in Europe for these exact requirements. We work a lot on this topic at the HZB and can therefore contribute a lot of knowhow for developing advanced empirical techniques and constructing new instrumentation specifically adapted for the research topic of battery materials.

Is that an opportunity for the HZB?
Yes, BESSY II is recognised in the synchrotron community as an energy synchrotron. Our strength lies in looking at the electronic properties of materials – such as how the charge carriers move, how materials change their properties and as a result develop new functionalities. It is exactly these effects that play a pivotal role in materials for energy and information technologies. And the nice thing is these are precisely the focal points of our own in-house research. The strong linkage between our in-house research and the operation of a synchrotron makes the HZB unique.

While BESSY II is a light source, at its core it is a particle accelerator. This means that accelerator development is also an important part of our research. What strategic topics will we contribute to during the new Helmholtz POF IV funding period?
One top task of our accelerator physics department is the operation and further development of BESSY II, as well as the development of the accelerator for our new BESSY III facility. If you combine this with an ambitious accelerator research programme that has a global profile, then the research and the operations cross-fertilise each other. One can devise concepts and develop them to a certain degree of maturity, to the point that they can then be tested in the equipment with a view towards using them for BESSY III.

We are establishing infrastructures for such research programmes, in which we collaborate with other Helmholtz Centres. This has great strategic importance. In addition, there is the aspect of promoting young talent: attractive research programmes attract talented young people who provide us with new ideas. Fresh, imaginative thinking is a prerequisite for more regimented areas of thought and endeavour.

Could you give us an example?
We are very active in the ARD programme of the Helmholtz Association to develop superconducting RF components. We can use these to manipulate accelerated electron bunches in such a way that the properties of the emitted X-ray beam can be adapted to the requirement of experiments.

> “We ask ourselves what modes of operation and experiments do we have that no other source offers, and can be adapted to meet a need that no other synchrotron covers.”

Do BESSY-VSR and bERLinPro also fit in here?
Yes, they do. We have reoriented the projects, and with support from the HZB Scientific Advisory Board and the HZB Supervisory Board we have found a new funding programme for implementation. With bERLinPro, we will be able to offer a new infrastructure through the POF programme that is not only ideal for our own research, but also offers our colleagues in the Helmholtz Association opportunities for conducting completely new experiments. That’s a nice prospect.

And how do things look with BESSY-VSR?
When the manufacturer of our RF cavities went bankrupt, we succeeded in arranging with the only remaining manufacturer to produce cavities for us within acceptable time and cost constraints. Once the BESSY-VSR demo module has been successfully built, we could even imagine BESSY-VSR and bERLinPro becoming more closely integrated, and prospectively merge them.

A project team began making concrete plans in October 2019 for a successor light source named BESSY III. What does the roadmap for this look like? And how much tailwind is the cause getting from outside the HZB?

The support is there. In 2018, tackling BESSY III was written into the HZB assessment as a top priority. We took this up immediately, for example by looking for a suitable site in order to have the option of a new building.

> "We do not simply want to build a synchrotron, but instead a large-scale research apparatus integrated in a laboratory environment with which we facilitate novel synchrotron research."

The support was then confirmed at the strategic review in January 2020. Expert opinion held that PETRA IV at DESY and BESSY III are equally important projects to the future of the Helmholtz Research Field Matter. Moreover, we also have strong support for this from the Helmholtz Association and the Federal Ministry of Education and Research (BMBF). BESSY III is on the current roadmap of the Helmholtz Association for Research Infrastructures, and the application has received unqualified support from the entire research sector. The project is also constantly on everyone's lips in the research community. We have seen the joy at workshops and conferences everywhere with which the launch of the project was received.

How is the community going to be involved in the planning? How will you make sure that we design a source that optimally meets the needs of research in Germany and Europe?

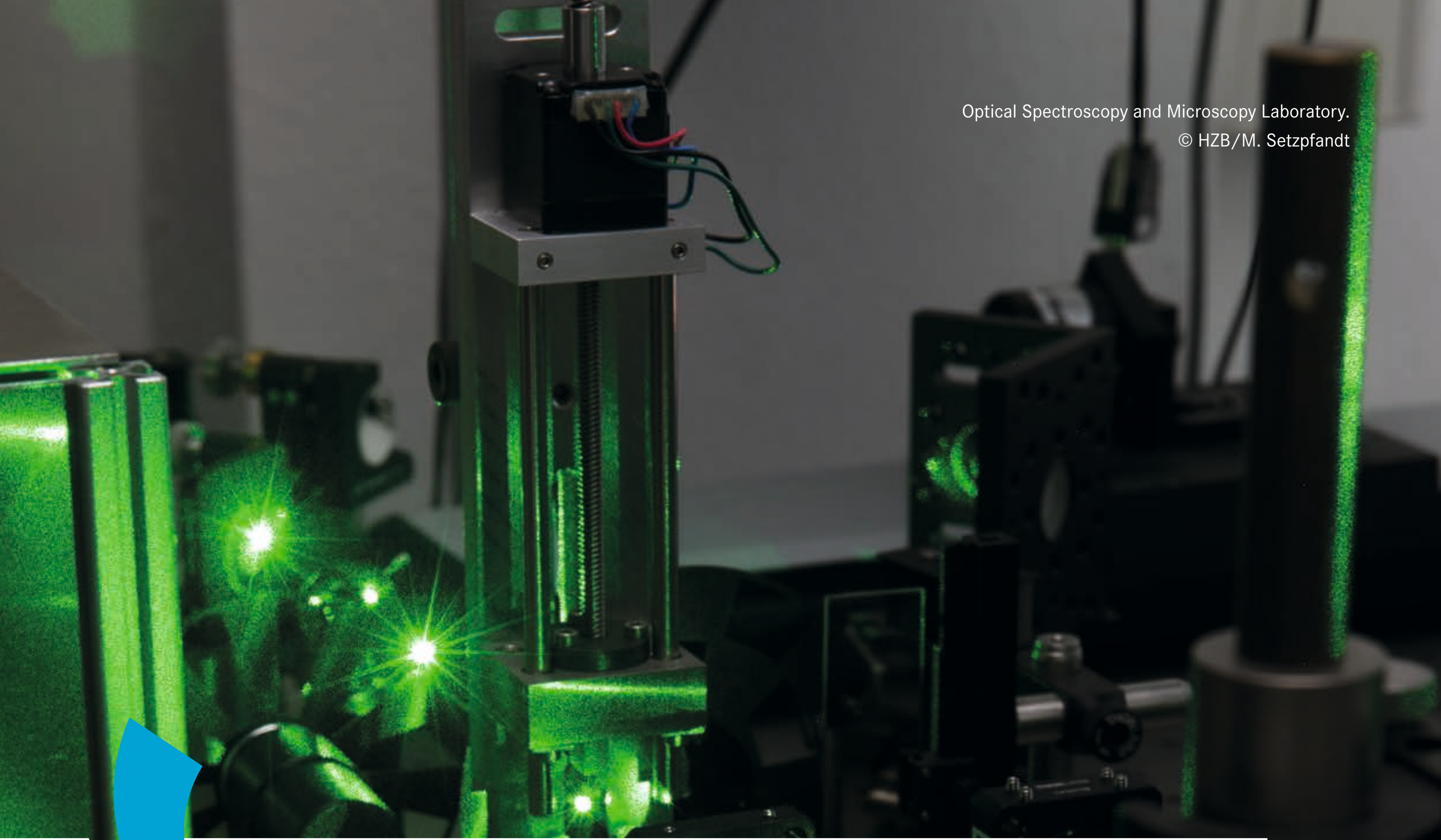
We are basing our planning on three inputs: firstly, on our own research; after all, this has just been evaluated with top marks. That means our in-house research is on the right path. Secondly: our partners from the Federal Institute for Materials Research and Testing (BAM), the German national metrology institute (PTB), the Max Planck Society, and the universities think and plan for the long term. This is reflected in their appointments. We ascertain the institutional needs from these as well. Thirdly, we see the needs arising from our user groups. This information flows into our planning process via workshops and through scientific expert groups.

At our international Foresight Workshops, we listen carefully to the broad user community. The expert groups are involved with specialised topics. We expect soft X-rays will be able to make an important contribution to this research. We exchange ideas with the leading experts in these fields about the current synchrotron experiments as well. Because we do not simply want to build a synchrotron, but instead a large-scale research apparatus integrated in a laboratory environment with which we facilitate novel synchrotron research. One example is the EMIL laboratory, which we have already connected directly to BESSY II. Advanced *in situ* and *in operando* measurement techniques enable us to enormously accelerate research on energy materials.

What opportunities for industrial collaboration are offered by BESSY II and will be offered by BESSY III?

Three aspects are important here. Firstly, we offer empirical measurements, i.e. analytic means for specific issues that a company cannot successfully address with conventional methods. The second opportunity is that we can develop something jointly with industrial partners, such components for the accelerator, microscopes, monochromators, and special analytical equipment. The third opportunity is that we are a customer and need something. In these cases we stimulate new development; we are a driving force for companies to develop something for us and then also bring this to market. 3-D printing is an example of one way to do this. This can be used to create cavities that no longer need to be milled from solid blocks of metal. BESSY III will therefore also be of interest to local companies as an exciting field of activity and be a driver of innovation.

The interview was conducted by Silvia Zerbe and Ina Helms.



Optical Spectroscopy and Microscopy Laboratory.
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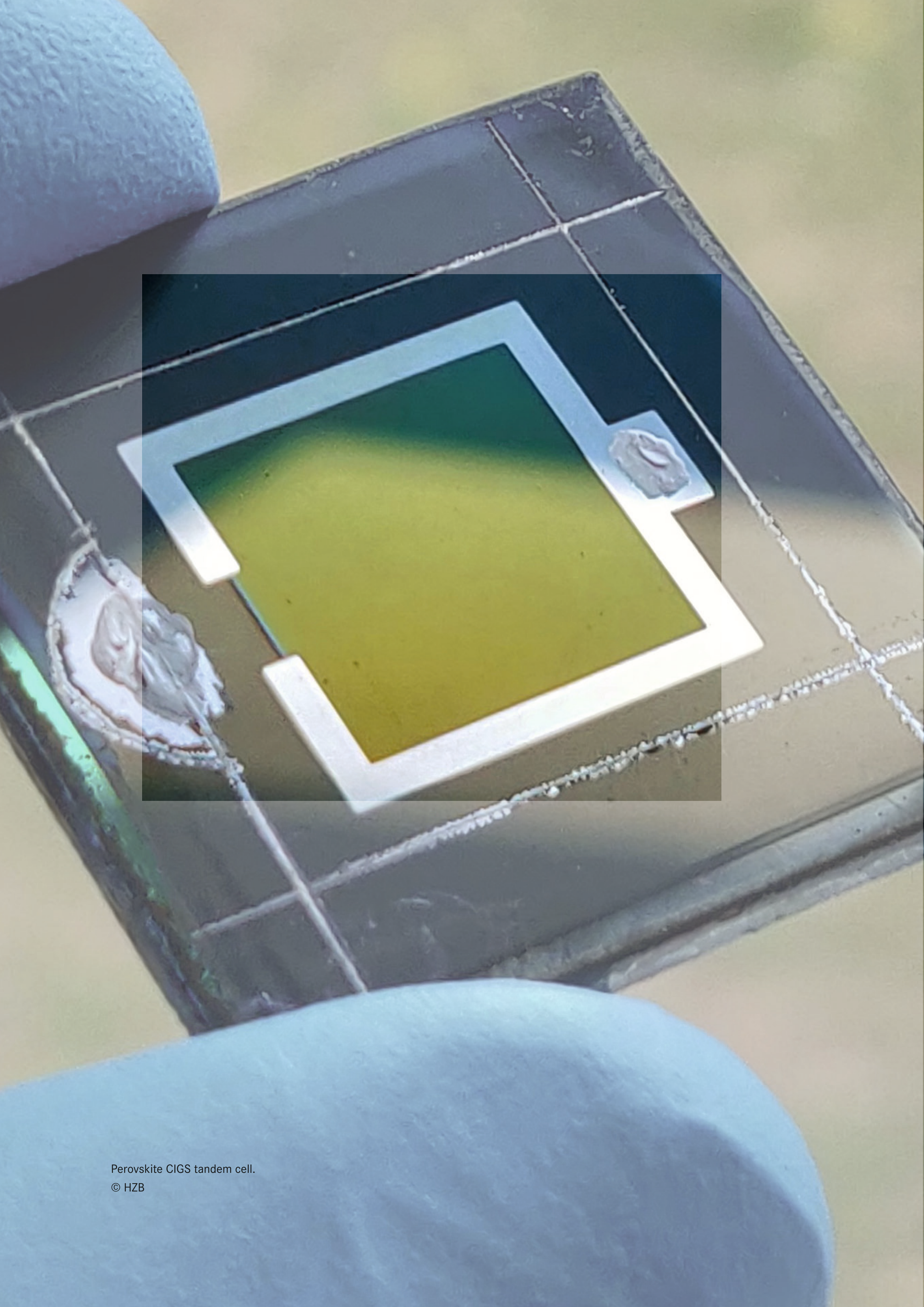
HIGHLIGHTS FROM OUR RESEARCH

In 2019 and 2020, a total of more than 1,900 articles were published in renowned journals by researchers from the HZB or by our visiting users with HZB participation. The 2019/2020 edition of Highlights presents a selection of these by research field, representing Energy, Information, Matter, and from user experiments. The short texts provide a quick impression of the diversity of research topics. **Each news item is accompanied by a more detailed text in the HZB Newsroom. You can also search for data and by keywords there.**

www.helmholtz-berlin.de/news



Perovskite CIGS tandem cell.
© HZB

ENERGY

WORLD RECORDS FOR TANDEM SOLAR CELLS WITH PEROVSKITES

The illustration shows schematically the structure of the tandem solar cell.
© HZB/ E. Köhnen

Solar cells made of two semiconductors with differing band gaps can achieve significantly higher efficiencies together as a tandem than each solar material on its own. This is because such tandem cells make more efficient use of the solar spectrum. In 2019-2020, HZB teams achieved new world records with tandem cells made of silicon and perovskite as well as CIGS and perovskite.

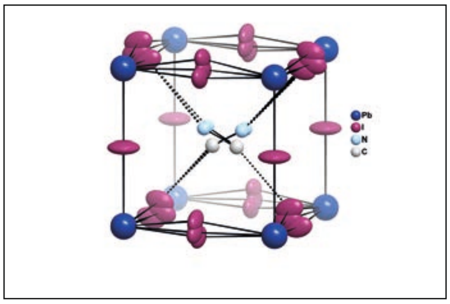
The tandem solar cell made of silicon and perovskite achieves an efficiency of 29.15 % and even without encapsulation exhibits stable performance over a period of 300 hours. Steve Albrecht's Young Investigator Group investigated physical processes at the interfaces and found how to improve the charge carrier transport. To do this, they developed with partners from Lithuania an intermediate layer of organic molecules that independently self-assembled into a monolayer. The work was published in Science.

The other world record tandem cell comprises semiconductors of perovskite and CIGS that are interconnected to form a **monolithic two-terminal tandem cell**. Thanks to the thin-film technologies used, such tandem cells can be produced on flexible film substrates. This tandem cell achieves a certified efficiency of 24.16 %. Moreover, it is also suitable for use in satellites, as it remains stable even under conditions found in space in the presence of strong radiation. Two patents have been filed for it. This work appeared in *Joule*.

Science 2020: Over 29%- efficient Monolithic Perovskite/Silicon Tandem Solar Cell Enabled by Enhanced Hole Extraction. Amran Al-Ashouri, Eike Köhnen, Bor Li, Artiom Magomedov, Hannes Hempel, Pietro Caprioglio, José A. Márquez, Anna Belen Morales-Vilches, Ernestas Kasparavicius, Joel A. Smith, Nga Phung, Dorothee Menzel, Max Grischek, Lukas Kegelmann, Dieter Skroblin, Christian Gollwitzer, Tadas Malinauskas, Marko Jošt, Gašper Mati[1], Bernd Rech, Rutger Schlatmann, Marko Topi[1], Lars Korte, Antonio Abate, Bernd Stannowski, Dieter Neher, Martin Stolterfoht, Thomas Unold, Vytautas Getautis, Steve Albrecht.
DOI: 10.1126/science.abd4016

JOULE (2020): Proton Radiation Hardness of Perovskite Tandem Photovoltaics. Felix Lang, Marko Jošt, Kyle Frohna, Eike Köhnen, Amran Al-Ashouri, Alan R. Bowman, Tobias Bertram, Anna Belen, Morales-Vilches, Dibyashree Koushik, Elizabeth M.Tennyson, Krzysztof Galkowski, Giovanni Landi, Mariadriana Creatore, Bernd Stannowski, Christian A. Kaufmann, Jürgen Bundesmann, Jörg Rappich, Bernd Rech, Andrea Denker, Steve Albrecht, Heinz-Christoph Neitzert, Norbert H. Nickel, Samuel D. Stranks.
DOI: 10.1016/j.joule.2020.03.006

PEROVSKITE SOLAR CELLS: POSSIBLE CAUSE FOR HIGH EFFICIENCIES UNCOVERED

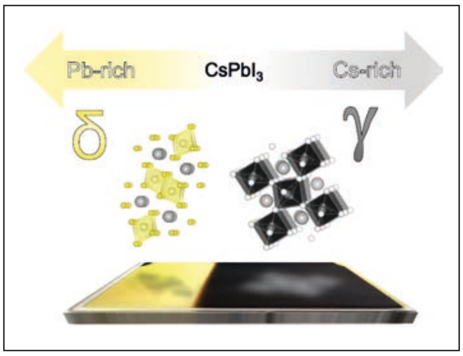


The drawing illustrates how organic methyl ammonium ions ($CH_3NH_3^+$) interact with the iodide ions. © HZB

Using crystallographic analyses at the Diamond Light Source (DLS) synchrotron source in the UK, an HZB team has demonstrated for the first time that hybrid perovskites crystallise without inversion centres. Interactions between the organic molecules and neighbouring iodine atoms can form ferroelectric domains that facilitate higher efficiencies in solar cells through further effects. This ferroelectric domain formation cannot take place in inorganic perovskites.

Angewandte Chemie International Edition (2019): Role of the Iodide–Methylammonium Interaction in the Ferroelectricity of $CH_3NH_3PbI_3$. J. Breternitz, F. Lehmann, S. A. Barnett, H. Nowell, S. Schorr. **DOI: 10.1002/anie.201910599**

INORGANIC PEROVSKITES FOR THIN-FILM SOLAR CELLS

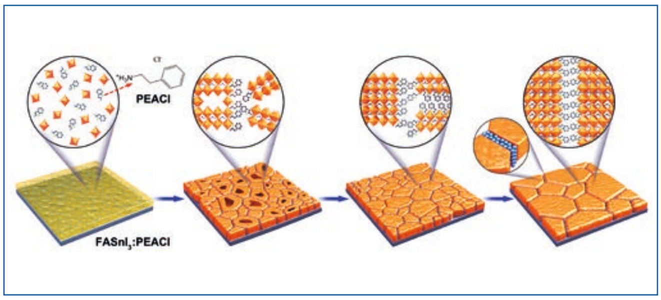


Thin films of C_sPbI_3 can also be produced at moderate temperatures by means of co-evaporation of caesium iodide and lead iodide. © HZB/J. Marquez-Prieto

A team at the Helmholtz-Zentrum Berlin has succeeded in producing inorganic perovskite thin-films at moderate temperatures through co-evaporation – obviating the need for post-curing at high temperatures. This makes it much easier to produce thin-film solar cells from this material. In contrast to the hybrid metal-organic perovskites, inorganic perovskites are thermally more stable.

Advanced Energy Materials (2019): Low Temperature Synthesis of Stable Y-$CsPbI_3$ Perovskite Layers for Solar Cells Obtained by High Throughput Experimentation. Pascal Becker, José A. Márquez, Justus Just, Amran Al[1]Ashouri, Charles Hages, Hannes Hempel, Marko Jošt, Steve Albrecht, Ronald Frahm, Thomas Unold. **DOI: 10.1002/aenm.201900555**

LEAD-FREE, STABLE PEROVSKITE SOLAR CELLS

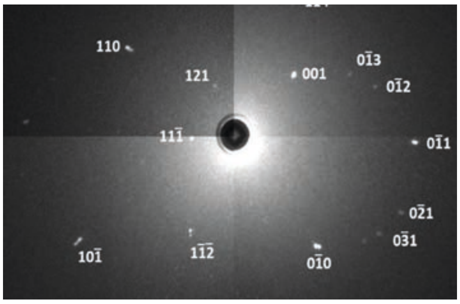


The figure shows the changes in the structure of FASnI3:PEACI films during treatment at different temperatures. © HZB/M. Li

Though the best perovskite solar cells achieve enormous efficiency, they contain toxic lead. Up to now, lead-free perovskite solar cells have only achieved lower efficiency, which also drops rapidly. A new study by an international collaboration has now shown how to produce stable perovskite layers containing tin instead of lead. Organic compounds protect the tin from oxidation and ensure stability.

ACS Energy Letters (2020): Tin halide perovskite films made of highly oriented 2D crystals enable more efficient and stable lead-free perovskite solar cells. Meng Li, Wei-Wei Zuo, Ying-Guo Yang, M. H. Aldamasy, Qiong Wang, Silver-Hamill Turren-Cruz, Shang-Lei Feng, Michael Saliba, Zhao-Kui Wang, Antonio Abate. **DOI: 10.1021/acsenergylett.0c00782**

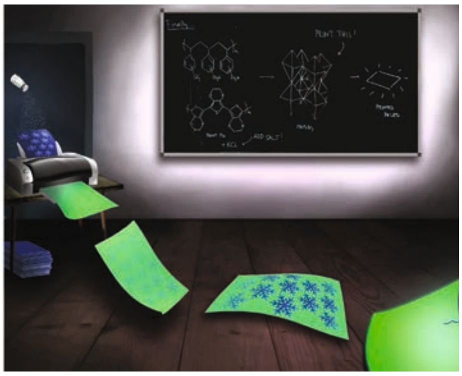
NEUTRONS REVEAL TWINNING IN HALIDE PEROVSKITES



The diffraction pattern was recorded with the Laue camera. © HZB

Solar cells based on hybrid halide perovskites achieve high efficiencies. These blended organic-inorganic semiconductors are usually produced as thin films of microcrystals. An investigation with the Laue camera at the BER II neutron source was now able to reveal that twinning also occurs at room temperature during crystallisation. This insight is helpful for optimising the manufacturing processes of halide perovskites.

Scientific Reports (2020): **Twinning in $MAPbI_3$ at room temperature uncovered through Laue neutron diffraction.** Joachim Breternitz, Michael Tovar, Susan Schorr. **DOI: 10.1038/s41598-020-73487-1**

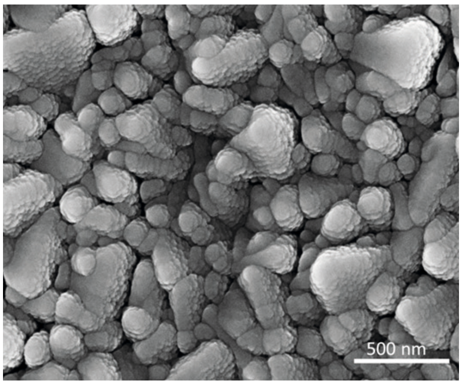


Graphical representation of the printing process for perovskite LEDs. © C. Rothkirch/HU Berlin

PEROVSKITE LEDS FROM A PRINTER

Researchers from the HZB and Humboldt-Universität zu Berlin have succeeded for the first time in producing light-emitting diodes (LEDs) from a hybrid perovskite semiconductor material using inkjet printing. This opens the door to broad application for such materials in many different electronic components. The team achieved the breakthrough with the help of a trick: "seeding" the surface with specific crystals.

Journal Materials Horizons (2020): **Finally, inkjet-printed metal halide perovskite LEDs – utilizing seed crystal templating of salty PEDOT:PSS.** Felix Hermerschmidt, Florian Mathies, Vincent R. F. Schröder, Carolin Rehermann, Nicolas Zorn Morales, Eva L. Unger, Emil. J. W. List-Kratochvil. **DOI: 10.1039/d0mh00512f**



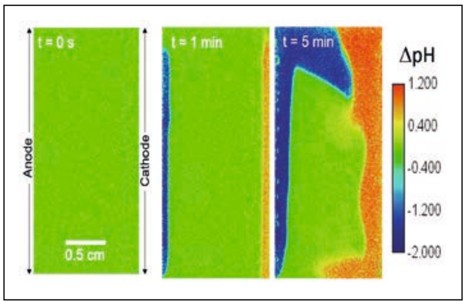
Scanning electron microscopy shows a molybdenum sulphide film that was applied at room temperature. © HZB

AMORPHOUS MOLYBDENUM SULPHIDE WORKS BEST

Efficient and inexpensive catalysts are needed for the production of solar hydrogen. Molybdenum sulphides are considered good candidates. Now a team at the HZB has established what processes take place in molybdenum sulphides during catalysis and why amorphous molybdenum sulphide on balance works best. "We can deduce from empirical data that degeneration due to separation and escape of the sulphur leads to formation of sulphur-depleted regions with islands of nanocrystalline MoS_2. These islands act as catalytically active particles", explains Fanxing Xi, who carried out the measurements as part of her PhD. These insights can help to further improve the activity and stability of this promising catalyst for hydrogen evolution in the process of water splitting, and to couple the material to an electrolyser powered by sunlight.

ACS Catalysis (2019): **Structural Transformation Identification of Sputtered Amorphous MoS_x as an Efficient Hydrogen-Evolving Catalyst during Electrochemical Activation.** Fanxing Xi, Peter Bogdanoff, Karsten Harbauer, Paul Plate, Christian Höhn, Jörg Rappich, Bin Wang, Xiaoyu Han, Roel van de Krol, Sebastian Fiechter. **Doi: 10.1021/acscatal.8b04884**

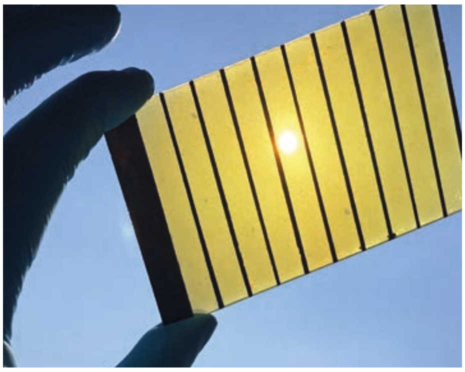
GREEN HYDROGEN: BUOYANCY EFFECTS DRIVE CONVECTION IN ELECTROLYTE



The local pH value changes over time (shown here in an electrolyte of 0.5 M K_2SO_4). © HZB

Hydrogen can be produced with neutral climate impact using sunlight. But there are still hurdles along the way from laboratory scale to large-scale implementation. Now a team at the HZB has developed a method to make the flow processes in the electrolyte visible and to simulate it reliably in advance with a model. The results are useful in support of the design and scale-up of the technology and were published in the renowned journal Energy and Environmental Science.

Energy & Environmental Science (2020): **In-situ Observation of pH Change during Water Splitting in Neutral pH Conditions: Impact of Natural Convection Driven by Buoyancy Effects.** Keisuke Obata, Roel van de Krol, Michael Schwarze, Reinhard Schomäcker, Fatwa F. Abdi. **DOI: 10.1039/D0EE01760D**



Scalable large-area $BiVO_4$ photoanode on FTO with Ni current collectors. © HZB

MEASURING THE STABILITY OF PHOTOELECTRODES

Solar energy can be used to split water - producing hydrogen, a versatile fuel, but high-quality photoelectrodes are necessary to achieve this. Unfortunately, the known materials tend to become unstable during the process and corrode. Now an international team at the HZB has studied the corrosion processes of high-quality $BiVO_4$ photoelectrodes. They observed the oxygen evolution reactions *in operando* (during electrolytic water splitting). The work demonstrated how the stability of the photoelectrodes and catalysts compare, and how they can be improved.

ACS Applied Energy Materials (2020): **Different Photostability of $BiVO_4$ in Near-pH-Neutral Electrolytes.** Siyuan Zhang, Ibbi Ahmet, Se-Ho Kim, Olga Kasian, Andrea M. Mingers, Patrick Schnell, Moritz Kölbach, Joohyun Lim, Anna Fischer, Karl J. J. Mayrhofer, Serhiy Cherevko, Baptiste Gault, Roel van de Krol, Christina Scheu. **DOI: 10.1021/acsaem.0c01904**

NANOPARTICLES DETECTED IN LITHIUM-SULPHUR BATTERIES

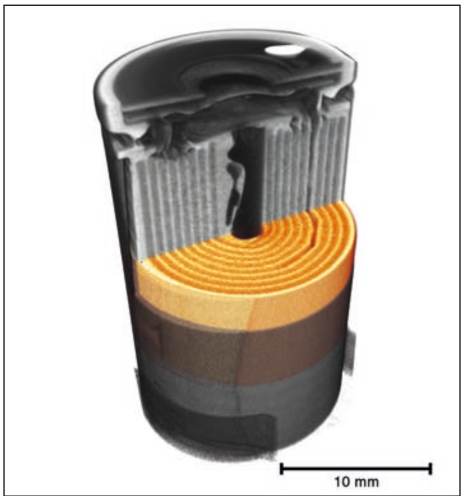
For the first time, an HZB team has used neutrons to precisely analyse how and where nanoparticles of lithium sulphide and sulphur are deposited on battery electrodes in the course of charging cycles. “We see that the deposition of lithium sulphide and sulphur does not take place inside the microporous carbon electrodes, but instead on the outer surface of the carbon fibres”, explains HZB researcher Sebastian Risse. These results can contribute to increasing the service life of lithium-sulphur batteries.

ACS Nano, (2019): **Operando Analysis of a Lithium/Sulfur Battery by Small Angle Neutron Scattering.** Sebastian Risse, Eneli Härk, Ben Kent, Matthias Ballauff. **DOI: 10.1021/acsnano.9b03453**

BATTERIES WITH SILICON ANODES: SURFACE STRUCTURES REDUCE CAPACITY

Theoretically, silicon anodes could store ten times more lithium ions than the graphite anodes used in commercial lithium batteries for many years. But so far, the capacity of silicon anodes drops significantly during the course of the charge-discharge cycles. Now an HZB team has used neutrons at BER II in Berlin and at the Institut Laue-Langevin in Grenoble to learn what happens on the surface of the silicon anode during charging and what processes reduce the capacity. They were able to observe how a blocking layer forms on the silicon surface during charging that hinders the penetration of lithium ions.

Energy Storage Materials (2019): Surface structure inhibited lithiation of crystalline silicon probed with operando neutron reflectivity. Arne Ronneburg, Marcus Trapp, Robert Cubitt, Luca Silvi, Sébastien Cap, Matthias Ballauff, Sebastian Risse. **DOI: 10.1016/j.ensm.2018.11.032**

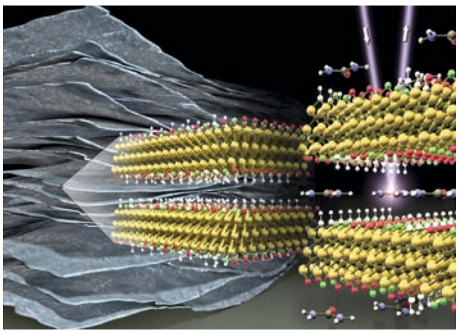


3-D view of a battery sliced open virtually.
© T. Arlt, I. Manke/HZB, R. Ziesche/UCL

AGEING OF LITHIUM BATTERIES ANALYSED

An international team has used neutron and X-ray tomography to study the dynamic processes taking place at the electrodes in lithium batteries that lead to power degradation. Using a new mathematical method, it was possible to virtually unroll the electrodes wound in a compact roll and thus to actually observe what happens at the electrodes. The study was published in Nature Communications.

Nature communications (2019): 4D imaging of lithium-batteries using correlative neutron and X-ray tomography with a virtual unrolling technique. Ralf F. Ziesche, Tobias Arlt, Donal P. Finegan, Thomas M. M. Heenan, Alessandro Tengattini, Daniel Baum, Nikolay Kardjilov, Henning Markoetter, Ingo Manke, Winfried Kockelmann, Dan J. L. Brett, Paul R. Shearing.
DOI: 10.1038/s41467-019-13943-3



MXenes are 2-D materials that are flakes formed of many layers (left) and suitable as pseudo-capacitors.
© HZB/M. Künsting

NEW 2-D MATERIALS WITH A TALENT FOR ENERGY STORAGE

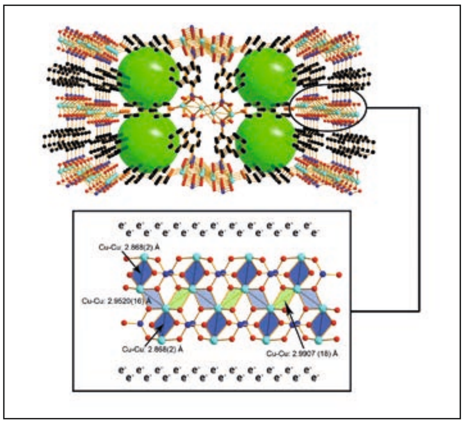
A new class of materials can store electrical energy very quickly. These are two-dimensional titanium carbides called MXenes. Like a battery, they store large amounts of electrical energy through electrochemical reactions - but unlike batteries, they can be charged and discharged in seconds. In collaboration with Drexel University, a team at the HZB has shown that the intercalation of urea molecules between the MXene layers can increase the capacity of these pseudo-capacitors by more than 50 per cent. At BESSY II, they have analysed which changes in the MXene surface chemistry are responsible for this after urea intercalation.

J. Phys. Chem. C (2020): Enhancement of Ti_3C_2 MXene Pseudocapacitance After Urea Intercalation Studied by Soft X-ray Absorption Spectroscopy. Ameer Al-Temimy, Babak Anasori, Katherine A. Mazzio, Florian Kronast, Mykola Seredych, Narendra Kurra, Mohamad-Assaad Mawass, Simone Raoux, Yury Gogotsi, Tristan Petit. **DOI: 10.1021/acs.jpcc.9b11766**

CHARGING AND DISCHARGING SILICON ELECTRODES

If silicon is used as a material for electrodes in lithium-ion batteries, it promises a significant increase in capacity. The shortcoming of this material is that it is easily damaged during charging and discharging. An HZB team has now succeeded for the first time in observing this process on crystalline silicon electrodes directly and in detail. Operando experiments at the BESSY II storage ring provided new insights into how fractures occur in silicon – and how the material can still be used advantageously.

Energy Storage Materials (2020): Morphological evolution of a single crystal silicon battery electrode during lithiation and delithiation: An operando phase-contrast imaging study. Arne Ronneburg, Markus Osenberg, Kang Dong, André Hilger, Eneli Härk, Luca Silvi, Ingo Manke, Matthias Ballauff, Sebastian Risse. **DOI: 10.1016/j.ensm.2020.06.007**

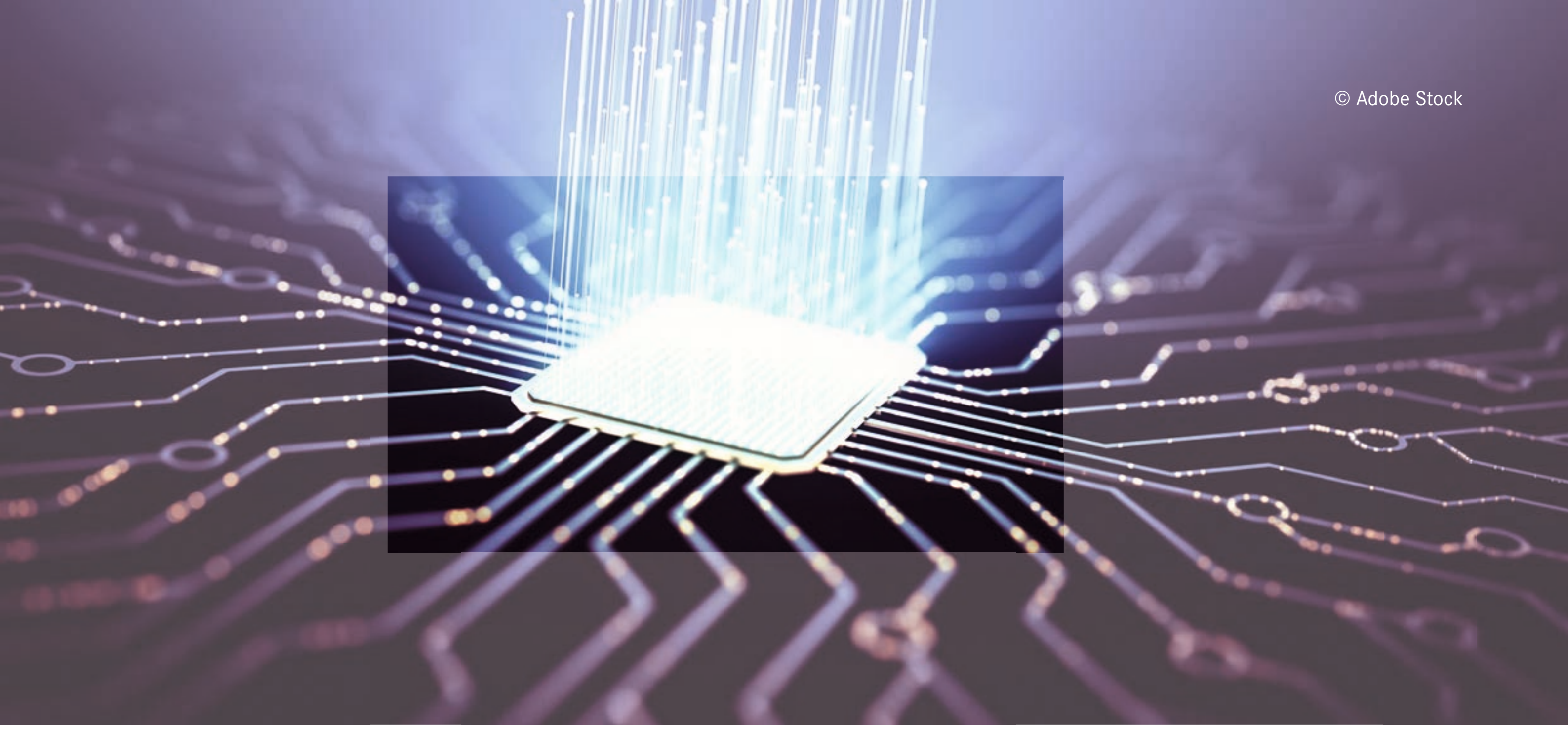


Structure of TUB75: the entire MOF architecture (above) and their conductive inorganic assembly unit (below). © HZB

NEW CLASS OF MATERIALS FOR TOMORROW'S ENERGY STORAGE

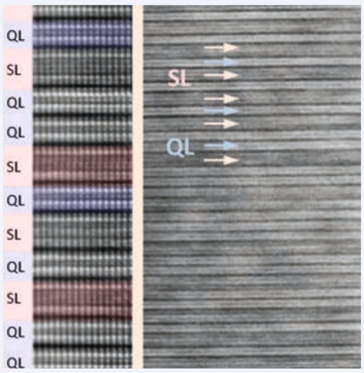
A group at the Technische Universität Berlin has created a new family of semiconductors, the properties of which were investigated by the Helmholtz-Zentrum Berlin (HZB). They christened the first representative TUB75. The material belongs to a class known as metal-organic frameworks, or MOFs for short. It could open up new prospects for energy storage.

Advanced Materials (2020): Phosphonate Metal–Organic Frameworks: A Novel Family of Semiconductors. Konrad Siemensmeyer, Craig A. Peeples, Patrik Tholen, Franz[1]Josef Schmitt, Bünyemin Çoşut, Gabriel Hanna, Gündoğ Yücesan. **DOI: 10.1002/adma.202000474**



INFORMATION

TOPOLOGICAL MATERIALS: SIGNAL TRANSMISSION WITHOUT LOSS



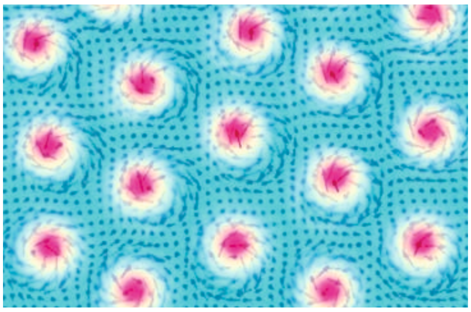
The image, taken with the transmission electron microscope, shows the superstructure formed by doping Bi_2Te_3 with manganese. © G. Springholz/Uni Linz

Experiments at BESSY II with magnetically doped topological insulators reveal new avenues for lossless signal transmission. The team headed by physicists Oliver Rader at the HZB and Gunther Springholz from the University of Linz has succeeded in precisely identifying what is known as the **magnetic energy gap** caused by the doping of the sample. Surprisingly, the gap was five times larger than theoretically predicted. The scientists found a simple reason for this result. “We now know that the doping is not disordered, but on the contrary produces what is known as a superstructure in the material that is similar to puff-pasty”, explains Springholz. “If these **self-organisation phenomena** are carefully exploited, completely new possibilities arise for assembling magnetic topological materials”, says Springholz.

In principle, the measured gap is already so large that it should facilitate a quantised **anomalous Hall Effect (QAHE)** near room temperature in corresponding components. Such a magnetic topological insulator could make it possible to realise the computing unit (Q-bit) of a topological quantum computer in conjunction with a superconductor.

Nature (2019): **Large magnetic gap at the Dirac point in Bi_2Te_3/$MnBi_2Te_4$ heterostructures.** E. D. L. Rienks, S. Wimmer, J. Sánchez-Barriga, O. Caha, P. S. Mandal, J. Růžička, A. Ney, H. Steiner, V. V. Volobuev, H. Groiss, M. Albu, G. Kothleitner, J. Michalička, S. A. Khan, J. Minár, H. Ebert, G. Bauer, F. Freyse, A. Varykhalov, O. Rader, G. Springholz. **DOI: 10.1038/s41586-019-1826-7**

MEASURING "DANCE PATTERNS" OF SKYRMIONS

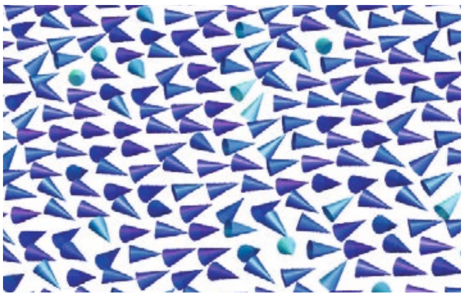


The illustration shows skyrmions in one of their self-oscillatory modes. Here they rotate clockwise. ©HZB/Y. Butt

In magnetic materials such as Cu_2OSeO_3, magnetic vortices called skyrmions can occur that might be important for energy-efficient data processing. Now, an HZB team at the VEKMAG station at BESSY II has developed a new technique to precisely measure these vortices. It was possible to observe three different self-oscillatory modes. With the help of a microwave field, the transitions from one self-oscillatory mode to another could be induced. This could be a way to control skyrmions.

Phys. Rev. Lett. (2019): Ferromagnetic Resonance with Magnetic Phase Selectivity by Means of Resonant Elastic X-Ray Scattering on a Chiral Magnet. S. Pöllath, A. Aqeel, A. Bauer, C. Luo, H. Ryll, F. Radu, C. Pfleiderer, G. Woltersdorf, C. H. Back. **DOI: 10.1103/PhysRevLett.123.167201**

GENERATING SUPERFERROMAGNETISM USING VOLTAGE

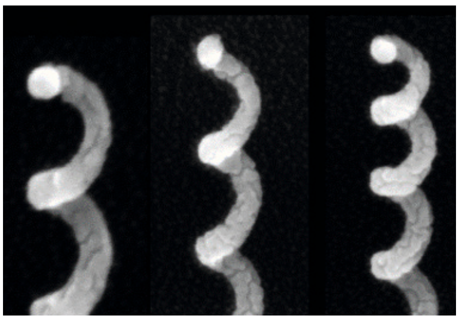


An electric field generates mechanical stresses in the barium-titanate lattice, which are transferred to the iron nanoparticles above. This causes the nanoparticles to align locally to a superferromagnetic region. © HZB

Together with international partners, an HZB team has observed a new phenomenon in iron nanograins on a ferroelectric substrate using the BESSY II light source. The magnetic moments of the iron grains align superferromagnetically as soon as an electric voltage is applied. The effect works at room temperature and could lead to new materials for IT components and data storage that consume less energy.

Physical Review Materials (2019): Switching on Superferromagnetism. A. Arora, L. C. Phillips, P. Nukala, M. Ben Hassine , A.A. Ünal, B. Dkhil, Ll. Balcells, O. Iglesias, A. Barthélémy, F. Kronast, M. Bibes, and S. Valencia. **DOI: 10.1103/PhysRevMaterials.3.024403**

DESIGN TOOL FOR CORKSCREW-SHAPED NANO-ANTENNAS

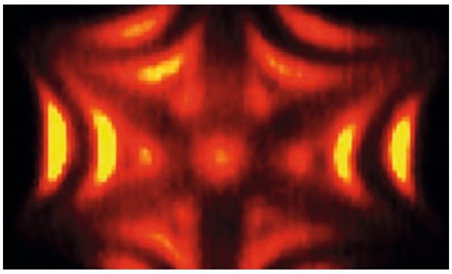


The nano-antennas are examined under an electron microscope via direct electron beam writing. © HZB

For the first time, an HZB team has mathematically formulated exactly how corkscrew-shaped nano-antennas interact with light. The mathematical tool can be used to calculate the appropriate geometry that a nano-antenna must have for specific applications in sensor and information technology. The work was carried out in the CoreLab for Electron Microscopy at the HZB.

Optica (2019): Resonant behavior of a single plasmonic helix. Katja Höflich, Thorsten Feichtner, Enno Hansjürgen, Caspar Haverkamp, Heiko Kollmann, Christoph Lienau, Martin Siles. **DOI: 10.1364/OPTICA.6.001098**

GERMANIUM TELLURIDE AT NANOSCALE

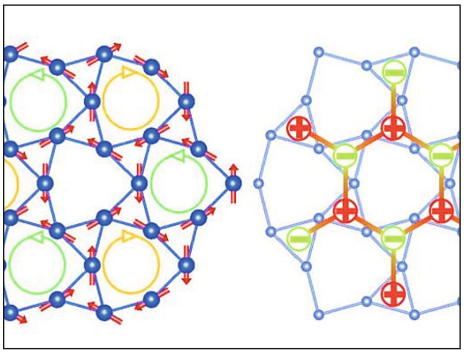


The Fermi surface of a GeTe Crystal (111) could be empirically determined at BESSY II. © HZB

Germanium telluride (GeTe) is an important material for the field of spintronics. Now, a German-Russian team at BESSY II has shown how the spin texture in GeTe single crystals can be switched by ferroelectric polarisation within individual nanodomains.

ACS Nano (2020): Atomic and Electronic Structure of a Multidomain GeTe Crystal. Alexander S. Frolov, Jaime Sánchez-Barriga, Carolien Callaert, Joke Hadermann, Alexander V. Fedorov, Dmitry Yu. Usachov, Alexander N. Chaika, Brian C. Walls, Kuanysh Zhussupbekov, Igor V. Shvets, Matthias Muntwiler, Matteo Amati, Luca Gregoratti, Andrei Yu. Varykhalov, Oliver Rader, Lada V. Yashina.
DOI: 10.1021/acsnano.0c05851

MAGNETIC MONOPOLES IN KAGOME SPIN ICE SYSTEMS

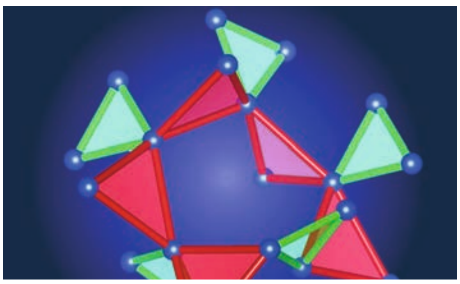


In HoAgGe, holmium spins occupy corners of triangles arranged in a kagome pattern. © Univ Augsburg

Magnetic monopoles are actually impossible. At low temperatures, however, what are known as quasiparticles can appear in certain crystals that behave like magnetic monopoles. Now, an international collaboration has proven that such monopoles also occur in a kagome spin ice system. Inelastic neutron scattering at the NEAT instrument of the BER II neutron source in Berlin was one of the techniques used. The results have been published in the journal Science.

Science (2020): Realization of the kagome spin ice state in a frustrated intermetallic compound. Kan Zhao, Hao Deng, Hua Chen, Kate A. Ross, Vaclav Petricek, Gerrit Günther, Margarita Russina, Vladimir Hutanu, Philipp Gegenwart.
DOI: 10.1126/science.aaw1666

THREE-DIMENSIONAL QUANTUM SPIN FLUID FOUND

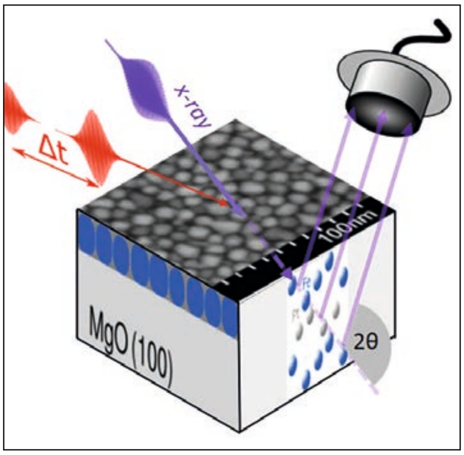


Two of the four magnetic interactions form a new three-dimensional network of triangles with common corners, known as a hyper-hyperkagome lattice, leading to the quantum spin liquid behaviour in $PbCuTe_2O_6$. © HZB

Quantum spin liquids are candidates for use in future information technologies. Until now, quantum spin liquids have usually only been found in one- or two-dimensional magnetic systems. Now, an international collaboration led by an HZB team has produced crystals of $PbCuTe_2O_6$ with neutron experiments. They found spin-fluid behaviour in three dimensions, due to what is called a hyper-hyperkagome lattice. The empirical data fit very well with theoretical simulations carried out at the HZB.

Nature Communications (2020): Evidence for a three-dimensional quantum spin liquid in $PbCuTe_2O_6$. S. Chillal, Y. Iqbal, H. O. Jeschke, J. A. Rodriguez-Rivera, R. Bewley, P. Manuel, D. Khalyavin, P. Steffens, R. Thomale, A. T. M. N. Islam, J. Reuther, B. Lake. **DOI: 10.1038/s41467-020-15594-1**

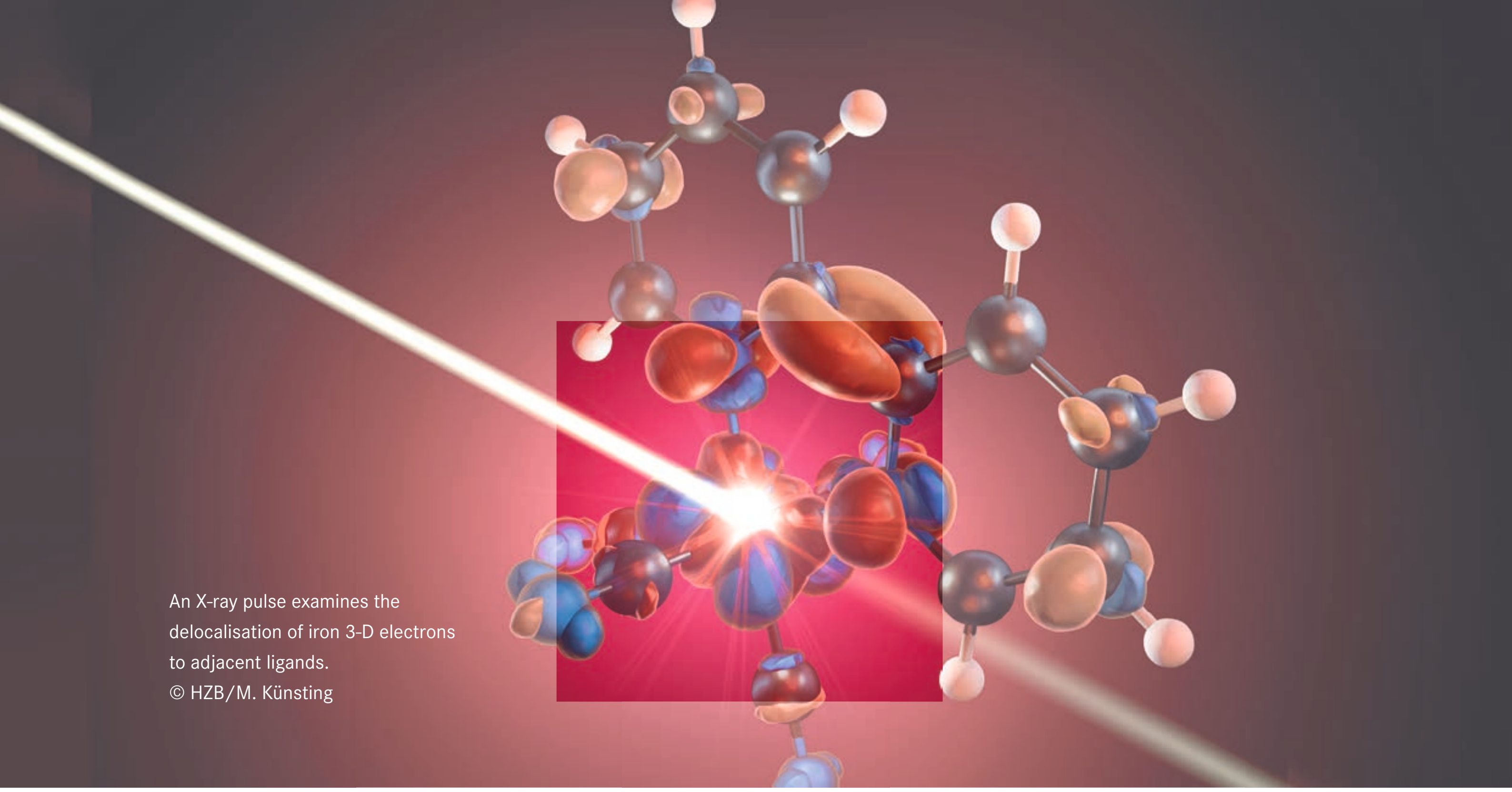
ROBUST HIGH-PERFORMANCE DATA STORAGE



This is how the experiment proceeded: two laser pulses strike the thin film of iron-platinum nano-granules at short intervals – the first laser pulse destroys the spin order, while the second laser pulse excites the now unmagnetised sample. An X-ray pulse then determines how the lattice expands or contracts.

The latest generation of magnetic hard-disk drives consists of magnetic thin-films made of invar that facilitate extremely robust and high data storage density. A technologically important material for these heat-resistant magnetic recording (HAMR) memories is a thin film of iron-platinum nanograins. An international team headed by the Joint Research Group of Matias Bargheer at the HZB and the University of Potsdam has now observed for the first time how a special spin-lattice interaction cancels out the thermal expansion of the crystal lattice in these iron-platinum thin films.

Science Advances (2020): **Spin stress contribution to the lattice dynamics of FePt.** A. von Reppert, L. Willig, J. Pudell, S. Zeuschner, G. Sellge, F. Ganss, O. Hellwig, J. A. Arregi, V. Uhlí[1], A. Crut, M. Bargheer. **DOI: 10.1126/sciadv.aba1142**



An X-ray pulse examines the delocalisation of iron 3-D electrons to adjacent ligands.
© HZB/M. Künsting

MATTER

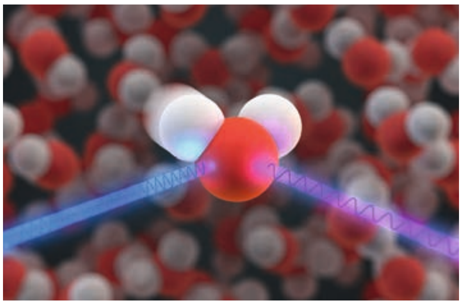
CHARGE TRANSFER WITHIN TRANSITION-METAL DYES ANALYSED

In dye-based solar cells, transition-metal complexes take care of converting light into electrical energy. Until now, it was assumed that spatial charge separation takes place within the molecule. An analysis at BESSY II shows that this is too simplistic a description of the process. For the first time, a team there has studied the **fundamental electronic processes** surrounding the metal atom and its ligands. "We were able to directly observe how the laser pulse depopulates the 3-D orbitals of the metal", explains Raphael Jay, doctoral student and first author of the study. These findings could contribute to the development of **new materials for dye-based solar cells**. Ruthenium complexes have been employed up to now in organic solar cells. However, ruthenium is a rare element and correspondingly expensive. Complexes of iron would be considerably less expensive, but exhibit high rates of recombination. Further investigations will show what is important in transition metal complexes so that light can be efficiently converted into electrical energy.

Angewandte Chemie International Edition (2019): covalency-driven preservation of local charge densities in a metal-to-ligand charge-transfer excited iron photosensitizer. Raphael M. Jay, Sebastian Eckert, Vinícius Vaz da Cruz, Mattis Fondell, Rolf Mitzner, Alexander Föhlisch. **DOI: 10.1002/anie.201904761**

News from the Helmholtz Field of Matter

WATER IS MORE HOMOGENEOUS THAN EXPECTED



Water molecules are excited with X-ray light (blue). Information about the hydrogen bridges can be obtained from light emitted (purple).

In order to explain the known anomalies in water, some researchers assume that water consists of a mixture of two phases even at ambient conditions. However, new X-ray spectroscopic analyses at BESSY II, the European Synchrotron Radiation Facility (ESRF) and the Swiss Light Source (SLS) show that this is not the case. At room temperature and atmospheric pressure, water molecules form a fluctuating network with an average of 1.74 ± 2.1 % donor and acceptor hydrogen bridge bonds per molecule, facilitating tetrahedral coordination between nearest neighbours.

PNAS 2019: Compatibility of quantitative X-ray spectroscopy with continuous distribution models of water at ambient conditions. Johannes Niskanen, Mattis Fondell, Sebastian Eckert, Raphael M. Jay, Annette Pietzsch, Vinicius Vaz da Cruz, Alexander Föhlisch. **DOI: 10.1073/pnas.1815701116**

HOW ELECTROLYTES BECOME METALLIC

An international team has developed an elegant new experiment at BESSY II to study the formation of a metallic conduction band in electrolytes. They prepared cryogenic solutions of liquid ammonia with various concentrations of alkali metals, then examined a microjet of the liquid with soft X-ray light. The transition from individual metal atoms in solution to a metallic compound is exhibited outwardly by the change in colour of the solution from blue to golden. They were now able to analyse this process in detail using measurement data from BESSY II. The work has been published in Science and appeared as the cover story.

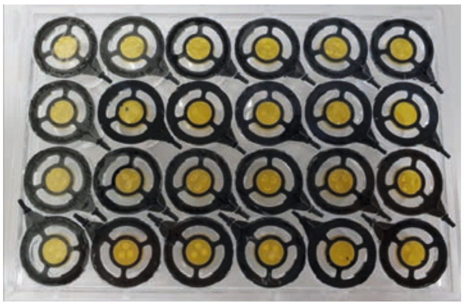
Science (2020): Photoelectron spectra of alkali metal–ammonia microjets: From blue electrolyte to bronze metal. Tillmann Buttersack, Philip E. Mason, Ryan S. McMullen, H. Christian Schewe, Tomas Martinek, Krystof Brezina, Martin Crhan, Axel Gomez, Dennis Hein, Garlef Wartner, Robert Seidel, Hebatallah Ali, Stephan Thürmer, Ondrej Marsalek, Bernd Winter, Stephen E. Bradforth, Pavel Jungwirth. **DOI: 10.1126/science.aaz7607**

ELECTRON-PHONON INTERACTIONS ANALYSED

How fast can a magnet change its orientation and what are the microscopic mechanisms? These questions are of utmost importance for the development of data storage devices and computer chips. Now, for the first time, an HZB team at BESSY II has succeeded in empirically observing the most important microscopic process of ultrafast magnetism. The methodology developed for this purpose can also be used to study interactions between spins and lattice vibrations in graphene, superconductors and other quantum materials.

Scientific Reports, 2019: Measuring the atomic spin-flip scattering rate by x-ray emission spectroscopy. Régis Decker, Artur Born, Robby Büchner, Kari Ruotsalainen, Christian Strahlman, Stefan Neppl, Robert Haverkamp, Annette Pietzsch, Alexander Föhlisch.
DOI: 10.1038/s41598-019-45242-8

NEW SAMPLE HOLDER FOR PROTEIN CRYSTALLOGRAPHY

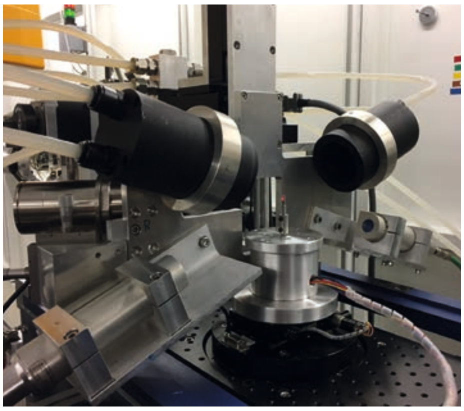


Up to three drops of protein solution can be applied to the sample holders. 24 sample holders are grouped on each plate each. © HZB

An HZB team has developed a novel sample holder that considerably facilitates the study of protein crystals. Proteins in solution crystallise on the sample holders themselves and can then be analysed directly on BESSY II's MX beamlines. This protects the tiny and very fragile protein crystals and saves steps of work. The sample holders are patented and can now be manufactured industrially.

J. Vis. Exp. (2019): An All-in-one Sample Holder for Macromolecular X-ray Crystallography with Minimal Background Scattering. Christian G. Feiler, Dirk Wallacher, Manfred S. Weiss. **DOI: 10.3791/59722**

WATCHING HOW METAL IS FOAMED



The rotary table operates extremely precisely at several hundred RPM about its axis. © HZB

Using a rotary table developed at the HZB, an international team at the Swiss Synchrotron Light Source (SLS) has achieved a new world record: at 208 three-dimensional X-ray tomographic images per second, they were able to document the dynamic processes involved in producing foamed aluminium from liquid aluminium. This new method, known as computer tomoscopy, might also provide insights into many other processes. For example, it could be used to investigate how materials change during laser welding or what happens when batteries overheat due to a short circuit (thermal runaway). The groups at the HZB and Paul Scherrer Institute (PSI) are now working on increasing the speed even further to enhance the temporal accuracy of the measurements.

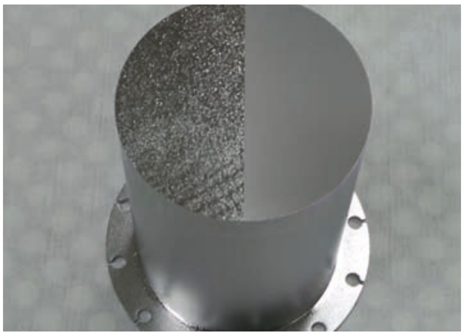
Nature communications (2019): Using X-ray tomoscopy to explore the dynamics of foaming metal. Francisco García-Moreno, Paul Hans Kamm, Tillmann Robert Neu, Felix Bülk, Rajmund Mokso, Christian Matthias Schlepütz, Marco Stampanoni, John Banhart. **DOI: 10.1038/s41467-019-11521-1**

SPECIAL ISSUE ON X-RAY METHODS

In the special issue of the **Philosophical Transactions of the Royal Society of London**, internationally renowned experts report on new developments in X-ray sources and ultrafast time-resolved experiments. Physicists from the HZB were invited to contribute.

- **Measurement of ultrafast electronic and structural dynamics with X-rays.** J. P. Marangos (ed.). **DOI: 10.1098/rsta/377/2145**
- **Recent Advances in Ultrafast X-ray Sources.** Robert Schoenlein, Thomas Elsaesser, Karsten Holldack, Zhirong Huang, Henry Kapteyn, Margaret Murnane, Michael Woerner. **DOI: 10.1098/rsta.2018.0384**
- **Chemical interactions and dynamics with femtosecond X-ray spectroscopy and the role of X-ray free-electron lasers.** Philippe Wernet. **DOI: 10.1098/rsta.2017.0464**

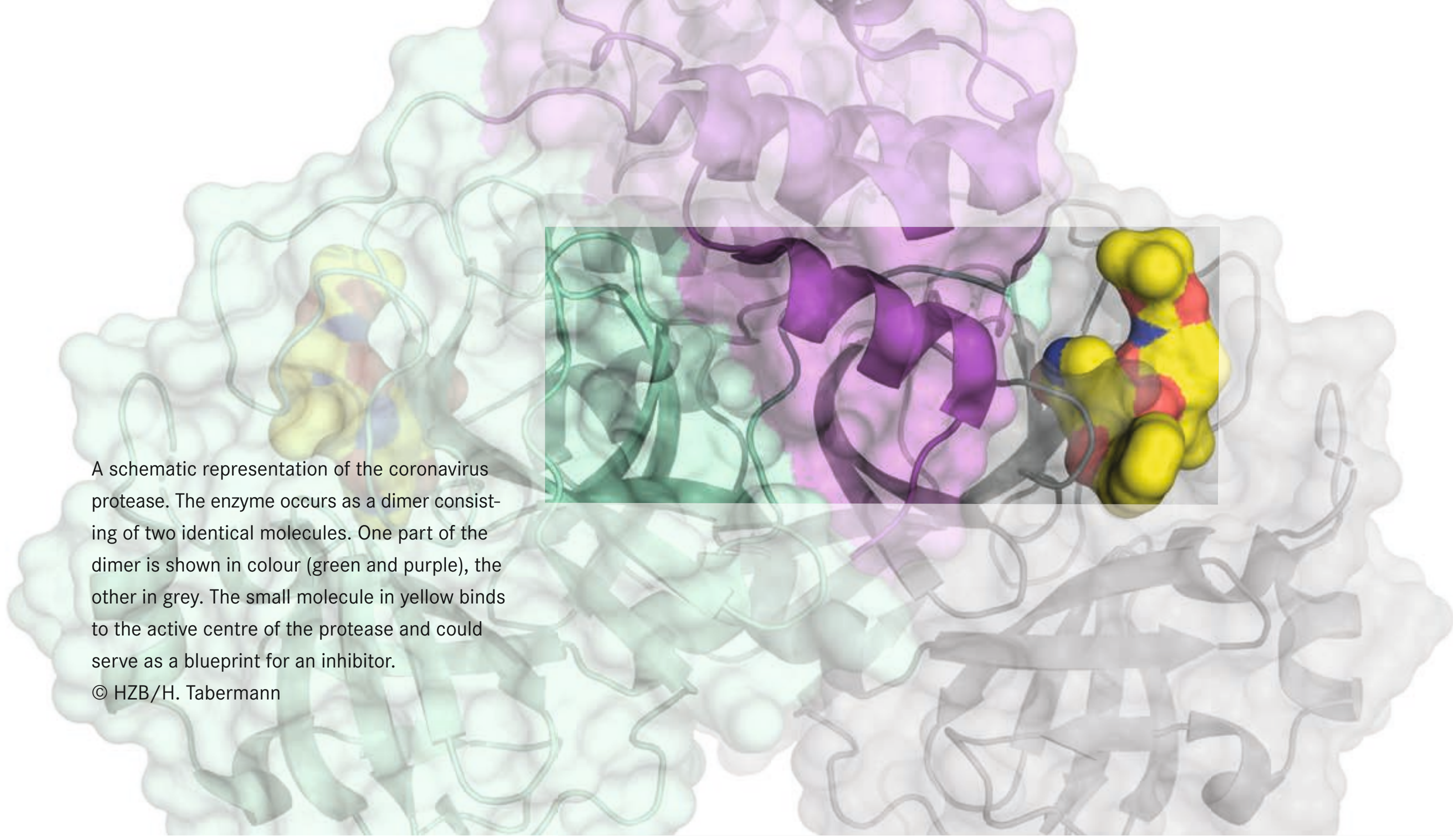
ALTERNATIVE MATERIAL FOR SUPERCONDUCTING HIGH-FREQUENCY CAVITIES TESTED



The photomontage shows a sample of pure niobium (left) and a sample coated with Nb_3Sn (right). © HZB

Superconducting high-frequency cavities can transport electron bunches in modern synchrotron sources and free-electron lasers with extremely high energy. At present, they are made of pure niobium. An international collaboration has now investigated what advantages a coating with niobium-tin confers compared to pure niobium. By combining different measurement methods, it could be shown that the coating process currently used for manufacturing the Nb_3Sn can still be improved.

Superconductor Science and Technology (2019): Critical fields of Nb_3Sn prepared for superconducting cavities. S. Keckert, T. Junginger, T. Buck, D. Hall, P. Kolb, O. Kugeler, R. Laxdal, M. Liepe, S. Posen , T. Prokscha, Z. Salman, A. Suter and J. Knobloch. **DOI:10.1088/1361-6668/ab119e**



A schematic representation of the coronavirus protease. The enzyme occurs as a dimer consisting of two identical molecules. One part of the dimer is shown in colour (green and purple), the other in grey. The small molecule in yellow binds to the active centre of the protease and could serve as a blueprint for an inhibitor.
© HZB/H. Tabermann

USER EXPERIMENTS

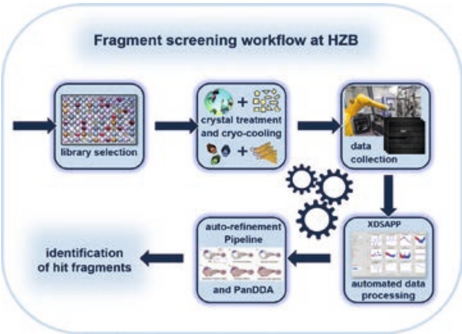
CORONAVIRUS SARS-COV-2: BESSY II DATA ACCELERATE THE SEARCH FOR DRUGS

Researchers worldwide are trying to find and develop **active substances against SARS-CoV-2**. The structural analysis of macromolecules that perform a function in the virus is important for this. Functions are closely related to the three-dimensional architecture of the macromolecule. If we know this three-dimensional architecture, we can identify specific targets for active substances. A team headed by Rolf Hilgenfeld from the University of Lübeck in early 2020 was already able to decode the **three-dimensional architecture of the main viral protease of SARS-CoV-2 at the MX beamlines of BESSY II**.

The main viral protease is involved in the replication of the virus. “We provide special fast-track access to our instruments for such highly topical questions”, says Manfred Weiss, who heads the macromolecular crystallography group at HZB. This results in concrete starting points for development of active substances. These could specifically dock onto weak points of the macromolecule and hinder its function.

Science (2020): **Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved α-ketoamide inhibitors.** Linlin Zhang, Daizong Lin, Xinyuanyuan Sun, Ute Curth, Christian Drosten, Lucie Sauerhering, Stephan Becker, Katharina Rox, Rolf Hilgenfeld. **DOI: 10.1126/science.abb3405**

NEW MOLECULE LIBRARY FOR ACTIVE SUBSTANCE SEARCH

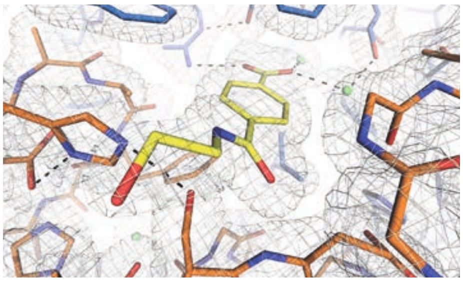


The fragment libraries, which the MX team built together with a group from the University of Marburg, are available to users at BESSY II. The diagram shows the sequence of the process of investigation. © HZB

In order to accelerate systematic development of drugs, the MX team at Helmholtz-Zentrum Berlin has built a new fragment library together with the Drug Design Group at the University of Marburg. It consists of 1,103 organic molecules that are potential building blocks for new active substances. The MX team has now validated this library in cooperation with the FragMAX group at MAX IV. The fragment library at HZB is available for research worldwide and is also playing a role in the search for active agents against SARS-CoV-2.

Structure (2020): F2X-Universal and F2X-Entry: Structurally Diverse Compound Libraries for Crystallographic Fragment Screening. Jan Wollenhaupt, Alexander Metz, Tatjana Barthel, Gustavo Lima, Andreas Heine, Uwe Mueller, Gerhard Klebe, Manfred S. Weiss. **DOI: 10.1016/j.str.2020.04.019**

“MOLECULAR SCISSORS” FOR PLASTIC WASTE



MHETase at work: MHET, part of the PET molecule, is broken down into the basic building blocks terephthalic acid and ethylene glycol. © HZB/G. Weber

A team from the University of Greifswald and the Helmholtz-Zentrum Berlin has decoded the structure of an important enzyme named MHETase at BESSY II. It was discovered in a bacterium and, together with a second enzyme, PETase, is able to break down the widely used plastic PET into its basic building blocks. The 3-D structure of MHETase has already enabled researchers to specifically optimise the activity of this enzyme in order to use it together with PETase for sustainable recycling of PET.

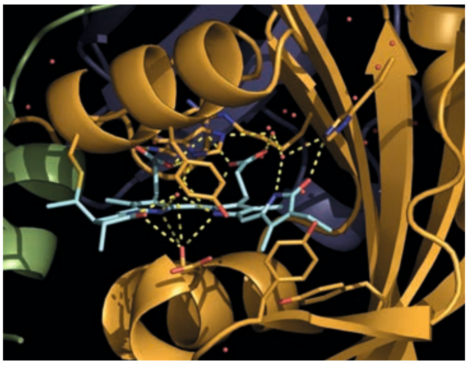
Nature Communications (2019): Structure of the plastic-degrading Ideonella sakaiensis MHETase bound to a substrate. G.J. Palm, L. Reisky, D. Böttcher, H. Müller, E.A.P. Michels, C. Walczak, L. Berndt, M.S. Weiss, U.T. Bornscheuer, G. Weber. **DOI: 10.1038/s41467-019-09326-3**

CANCER RESEARCH: BINDING MECHANISMS OF ACTIVE SUBSTANCES DECIPHERED

The DNA of tumour cells is altered from that of normal body cells. How such changes can be prevented or inhibited is an exciting area of research with huge relevance for the development of cancer treatments. An interdisciplinary team has now used protein crystallography at BESSY II to analyse the possible binding mechanisms of certain therapeutic substances from the group of tetrazole hydrazides to a crucial protein in the cell. A detailed evaluation revealed not only the three-dimensional architecture of this substance class, but also where exactly on the target molecule the active substances had docked. These insights help in the development of active substances.

ChemMedChem (2019): Structure-based screening of tetrazolylhydrazide inhibitors vs. KDM4 histone demethylases. Piotr H. Małecki, Nicole Rüger, Martin Roatsch, Oxana Krylova, Andreas Link, Manfred Jung, Udo Heinemann, Manfred S. Weiss. **DOI: 10.1002/cmdc.201900441**

INSIGHT INTO THE EYE OF PLANTS



A bilin pigment within the 3-D structure of a phyto-chrome molecule has been shown to be able to accept a photon. © J. Hughes

Plants use light not only for photosynthesis. Although the plant cell has no eyes, it can still perceive light and thus its environment. Phytochromes, certain turquoise-coloured proteins, play the central role in this, but exactly how they function is still unclear. Now, the team headed by plant physiologist Jon Hughes (Justus Liebig University Gießen) has been able to decode the three-dimensional architecture of various plant phytochrome molecules at BESSY II. This shows how light changes the structure of the phytochrome, causing the cell to transmit the light signal for guiding development of the plant.

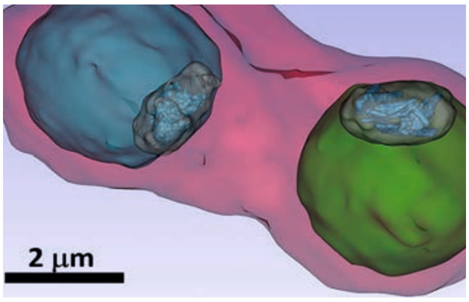
Nature Plants (2020): Structural insights into photoactivation and signalling in plant phytochromes. Soshichiro Nagano, Kaoling Guan, Sintayehu Manaye Shenkutie, Christian Feiler, Manfred Weiss, Anastasia Kraskov, David Buhrke, Peter Hildebrandt, Jon Hughes. **DOI: 10.1038/s41477-020-0638-y**

NANOPARTICLES CAN ALTER CELLS

Nanoparticles easily penetrate cells. How they distribute themselves there and what they do have now been shown for the first time by high-resolution 3-D microscopy images taken at the BESSY II and ALBA synchrotron light sources. Certain nanoparticles preferentially accumulate in particular organelles of the cell. This can increase the energy turnover of the cell. “The cell looks like it has run a marathon – obviously it costs energy to take up such nanoparticles”, says lead author James McNally.

ACS Nano (2020): Cells Undergo Major Changes in the Quantity of Cytoplasmic Organelles after Uptake of Gold Nanoparticles with Biologically Relevant Surface Coatings. Burcu Kepsutlu, Virginia Wycisk, Katharina Achazi, Sergey Kapishnikov, Ana Joaquina Pérez-Berná, Peter Guttmann, Antje Cossmer, Eva Pereiro, Helge Ewers, Matthias Ballauff, Gerd Schneider, James G. McNally. **DOI: 10.1021/acsnano.9b09264**

X-RAY ANALYSIS WITH BESSY II SHOWS HOW MALARIA AGENTS FIGHT PATHOGENS

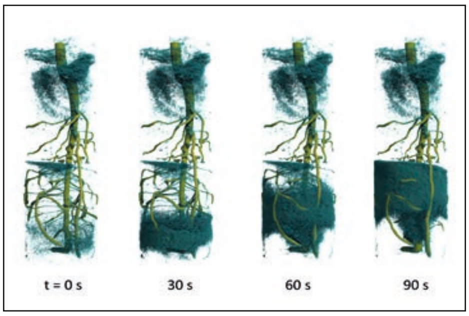


After staining, the plasmodia (blue and green) in the blood cell reveal many details, among others the vacuole © S. Kapishnikov

Malaria is one of the most devastating infectious diseases world-wide. Now, an international team has been able to study malaria pathogens in red blood cells under natural conditions using X-ray microscopy at BESSY II and the synchrotron sources ALBA and ESRF. The infected blood cells were mixed with different concen-trations of the active substance bromoquine from the quinoline family. Evaluation of the results shows the mechanisms by which the active substances attack the pathogens. These investigations can also be carried out with other active substances from the quinoline and artemisinin families and thus be used to improve malaria therapies.

PNAS (2019): Mode of action of quinoline antimalarial drugs in red blood cells in-fected by Plasmodium falciparum, revealed in-vivo. Sergey Kapishnikov, Trine Staalsø, Yang Yang, Jiwoong Lee, Ana J. Perez-Berna, Eva Pereiro, Yang Yang, Stephan Werner, Peter Guttmann, Leslie Leiserowitz, and Jens Als-Nielsen. **DOI: 10.1073/pnas.1910123116**

FASTER THAN EVER BEFORE: NEUTRON TOMOGRAPHY SHOWS HOW ROOTS “DRINK”



Time-resolved 3-D neutron tomography shows the rise of deuterated water in the root system of a lupine plant. © C. Tötzke/University of Potsdam

A team from Potsdam, Berlin, and Grenoble was able to use ultrafast 3-D neutron imaging to visualise the transport of water in soil and the subsequent uptake by roots of lupines. The ultrafast neutron tomography developed at the HZB produces a complete 3-D image every 1.5 seconds, seven times faster than before. “The tomographic method makes it possible to record the water flows in the soil and in the roots over time”, says Christian Tötzke. “These insights help to develop strategies for more efficient and sustainable use of water and fertiliser in the cultivation of crops.” The measurements were taken at the neutron source of the Institut Laue-Langevin in Grenoble, France. The method is in principle also useful for analysis of transport processes in other materials.

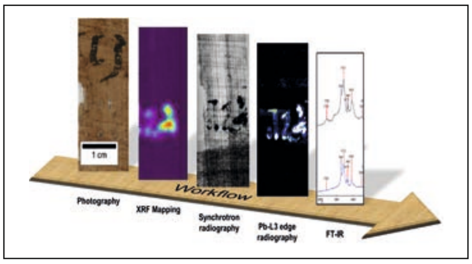
Published as a special recommendation of the editor in Optics Express (2019): What comes NeXT? – High-Speed Neutron Tomography at ILL. C. Tötzke, N. Kardjilov, N. Lenoir, I. Manke, S.E. Oswald, A. Tengattini. **DOI: 10.1364/OE.27.028640**

SEE, SMELL, TASTE: HOW BIOMOLECULES FUNCTION IN SENSORY CELLS

A team has analysed how the biomolecule rhodopsin changes after activation by light. Rhodopsin plays a central role in vision, but is also a prototype for receptors in other sensory organs. A newly developed infrared spectrometer at BESSY II has made it possible to conduct this investigation under natural conditions for the first time. With the new method, fast irreversible reactions can be observed with a single measurement. Until now, thousands of such reactions had to be evaluated to achieve this. However, many biological processes are irreversible and cannot be cyclically repeated.

Journal of Physical Chemistry Letters (2019): Féry Infrared Spectrometer for Single-Shot Analysis of Protein Dynamics. Eglof Ritter, Ljiljana Puskar, So Young Kim, Jung Hee Park, Klaus Peter Hofmann, Franz Bartl, Peter Hegemann, Ulrich Schade. **DOI: 10.1021/acs.jpclett.9b03099**

ARCHAEOLOGY AT BESSY II: “SECRET INK” REVEALED ON ANCIENT PAPYRUS FROM THE NILE

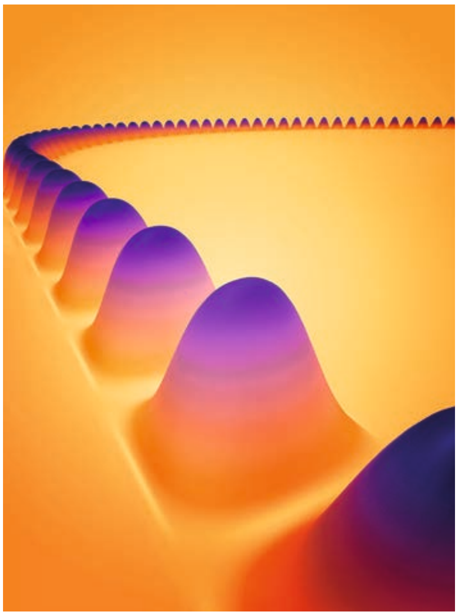


Examination of ancient papyrus with a supposed blank space. © HZB

The ancient Egyptians wrote many documents on pieces of papyrus, which were then carefully rolled or folded. Thousands of years later, however, it is impossible to unroll or unfold these valuable testimonies without destroying them. At BESSY II, however, this is achieved non-destructively through X-ray analyses and subsequent computer processing of the data, allowing the documents to be virtually unrolled or unfolded. At BESSY II’s BAMline, an interdisciplinary team has now succeeded in identifying traces of ink on an apparently empty piece of papyrus. It came from a collection excavated on the Nile island of Elephantine. The researchers not only discovered what kind of ink was used for the inscription, they also succeeded in making parts of the characters visible on the papyrus. The research team included experts from the Egyptian Museum and Papyrus Collection, from Berlin universities, and the Helmholtz-Zentrum Berlin.

Journal of Cultural Heritage (2019): **Absorption Edge Sensitive Radiography and Tomography of Egyptian Papyri.** T. Arlt, H.-E. Mahnke T. Siopi, E. Menei, C. Aibéo, R.-R. Pausewein, I. Reiche, I. Manke, V. Lepper. **DOI: 10.1016/j.culher.2019.04.007**

GUIDEPOST FOR SPIN WAVES



A spin wave propagates along a magnetic domain wall. © HZDR/Juniks

Waves of regularly oriented spins can propagate like electrical charges and transport information in the process. Significantly less heat is generated in the process. However, in order to be able to use them, spin waves must have a very short wavelength - and be able to be guided.

A team of researchers headed by Sebastian Wintz and Volker Sluka from the Helmholtz-Zenrum Dresden-Rossendorf and Markus Weigand from the HZB has succeeded in meeting both requirements for the first time. By exciting a combination of thin platelets having certain magnetic properties using high-frequency magnetic fields, they were able to generate waves with wavelengths of as little as around 100 nanometres. To do this, the researchers used domain walls: boundary regions between domains that have differently oriented spins. The team also found a way to keep spin waves within these walls - and thus control them. Using a powerful X-ray microscope at the HZB operated by the Max Planck Institute for Intelligent Systems based in Stuttgart, it was shown that the waves can even travel in a curve. This is a further step towards the development of novel, particularly energy-efficient computer chips.

Nature Nanotechnologies (2019): **Emission and Propagation of Multi-Dimensional Spin Waves in Anisotropic Spin Textures.** V. Sluka, T. Schneider, R. A. Gallardo, A. Kakay, M. Weigand, T. Warnatz, R. Mattheis, A. Roldan-Molina, P. Landeros, V. Tiberkevich, A. Slavin, G. Schütz, A. Erbe, A. Deac, J. Lindner, J. Raabe, J. Fassbender, S. Wintz. **DOI: 10.1038/s41565-019-0383-4**

USER OPERATIONS AT BER II

On 11 December 2019, the operation of the BER II research reactor ended after 46 years. Thanks to the early announcement of the closure by its supervisory board in 2013, the HZB succeeded in focussing it on research into energy materials and the advanced development of the BESSY II electron storage ring. BER II is to be dismantled over the next few years. The instruments have been and will be successively transferred to other neutron sources – nationally in preference to being transferred to international centres – in order to preserve them for continued scientific use.

BOROPHOSPHATES FOR EFFICIENT WATER SPLITTING

The deep pink crystals considerably increase the reaction efficiency. © TU Berlin

Hydrogen is one of the most important building blocks for the post-fossil-fuel age. It can be produced through electrocatalysis in a carbon-neutral way from water and green energy. This happens in two steps: the oxygen reaction, in which water is split into its components oxygen and hydrogen, and the hydrogen reaction, in which the hydrogen ions are converted into gaseous hydrogen. The electrode material and its catalytic properties are of great importance in this process. A team from the Technische Universität Berlin has now investigated the alkali metal compound cobalt borophosphate as a potential catalyst material. To do this, they also recorded its X-ray absorption spectra at the BESSY II synchrotron source. The result of their experiments was surprising: the porous, deep pink crystals are capable of increasing the efficiency of both these partial reactions for a long period of time without degrading. This abundant material thus facilitates design of simple, cost-effective, and durable systems for water splitting.

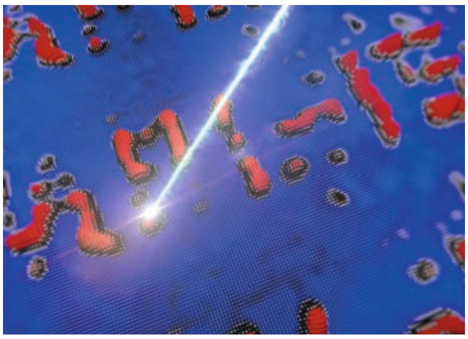
En. Envir. Science, impact: 33, citations: 29 (2019): Helical cobalt borophosphates to master durable overall water-splitting. Menezez, W.P.; Indra, A.; Zaharieva, I.; Walter, C.; Loos, S.; Hoffmann, S.; Schlögl, R.; Dau, H.; Driess, M. **DOI: 10.1039/c8ee01669k**

NOT ALL CRYSTALS CAN BE FORCED TO BE FERROMAGNETIC

The tiny magnetic moments in solids can normally be aligned with an external magnetic field so that the sample eventually becomes ferromagnetic. But this does not apply to every material. A team has now studied crystals of a uranium compound with neutrons under extremely high magnetic fields and observed much more complex behaviour. The experiments took place at HZB's BER II neutron source in the High-Field Magnet, which can generate a constant magnetic field of up to 26 tesla. This is about 500,000 times stronger than the Earth's magnetic field. Further experiments with pulsed magnetic fields of up to 45 tesla were conducted at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR).

Phys. Rev. Research (2020): Noncollinear magnetic structure in U2Pd2In at high magnetic fields. K. Prokeš, M. Bartkowiak, D. I. Gorbunov, O. Prokhnenko, O. Rivin, P. Smeibidl. **DOI: 10.1103/PhysRevResearch.2.013137**

NEW INTERACTION BETWEEN LIGHT AND MATTER



A focussed soft X-ray beam writes numerous magnetic vortices that together form the term "MPI-IS". © A. Posada, F. Groß/MPI-IS

A Sino-German team headed by Gisela Schütz from the Max Planck Institute for Intelligent Systems MPI has discovered a new interaction between light and matter at BESSY II. They succeeded in creating nanometre-sized magnetic vortices in a magnetic layer. These are called skyrmions, which are of interest for future information technologies.

Nature communications (2020): Creating zero-field skyrmions in exchange-biased multilayers through X-ray illumination. Yao Guang, Iuliia Bykova, Yizhou Liu, Guoqiang Yu, Eberhard Goering, Markus Weigand, Joachim Gräfe, Se Kwon Kim, Junwei Zhang, Hong Zhang, Zhengren Yan, Caihua Wan, Jiafeng Feng, Xiao Wang, Chenyang Guo, Hongxiang Wei, Yong Peng, Yaroslav Tserkovnyak, Xiufeng Han & Gisela Schütz. **DOI: 10.1038/s41467-020-14769-0**

FORMATION OF A 2-D META-STABLE OXIDE IN REACTIVE ENVIRONMENTS

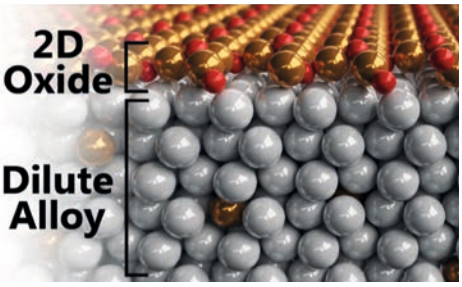


Illustration of the $Cu_x O_y$ structure described, formed on AgCu in oxidising environments. © (2020) ACS Publishing

The chemical behaviour of solid surfaces plays an important role in many applications involving catalysis, chemical sensors, fuel cells, and electrodes. A team of researchers at the Max Planck Institute for Chemical Energy Conversion has now described a phenomenon at the BESSY II synchrotron radiation source that can occur when metal alloys are exposed to reactive environments.

ACS Applied Materials & Interfaces 12(20): **Formation a 2D meta-stable oxide by differential oxidation of AgCu alloys.** Schweinar, K., Beeg, S., Hartwig, C., Rajamathi, C.R., Kasian, O., Piccinin, S., Prieto, M.J., Tanase, L.C., Gottlob, D.M., Schmidt, T., Raabe, D., Schlögl, R., Gault, B., Jones, T.E., Greiner, M.T. (2020).
DOI: 10.1021/acsami.0c03963

NEW MATERIALS INCREASE EFFICIENCY IN ETHANOL FUEL CELLS

The material consists of Nafion with embedded nanoparticles. © B.Matos/IPEN

A research group from Brazil together with an HZB team has investigated a novel composite membrane for ethanol fuel cells. It consists of a sulfonated tetrafluoroethylene-based fluoropolymer-copolymer named Nafion in which titanate nanoparticles are embedded by melt extrusion. At BESSY II, the researchers were able to observe how the nanoparticles are distributed in the Nafion matrix and how they increase the conductivity of protons.

Journal of Membrane Science (2020): **Properties and DEFC tests of Nafion-Functionalized titanate nanotubes composite membranes prepared by melt-extrusion.** B.R. Matos, C.A. Goulart, B. Tosco, J.S. da Silva, R.A. Isidoro, E.I. Santiago, M. Linardi, U. Schade, L. Puskar, F.C. Fonseca, A.C. Tavares.
DOI: 10.1016/j.memsci.2020.118042

SPECIAL PRIZES AND AWARDS

2019

Prof. Steve Albrecht received the Berlin Wissenschaftspreis science award for young researchers for his research on novel tandem solar cells and was also awarded the Karl Scheel Prize of the German Physical Society (DPG).

Dr. Godehard Wüstefeld was honoured with the Horst Klein Research Award of the German Physical Society for his outstanding contributions to accelerator research.

Dr. Eneli Härk was honoured with a medal at the International Association of Advanced Materials, IAAM.

Prof. Klaus Lips and **Prof. Jens Anders** received the 2019 HZB Technology Transfer Award for their project "EPR-on-a-Chip, a revolution in spin-based analytics".

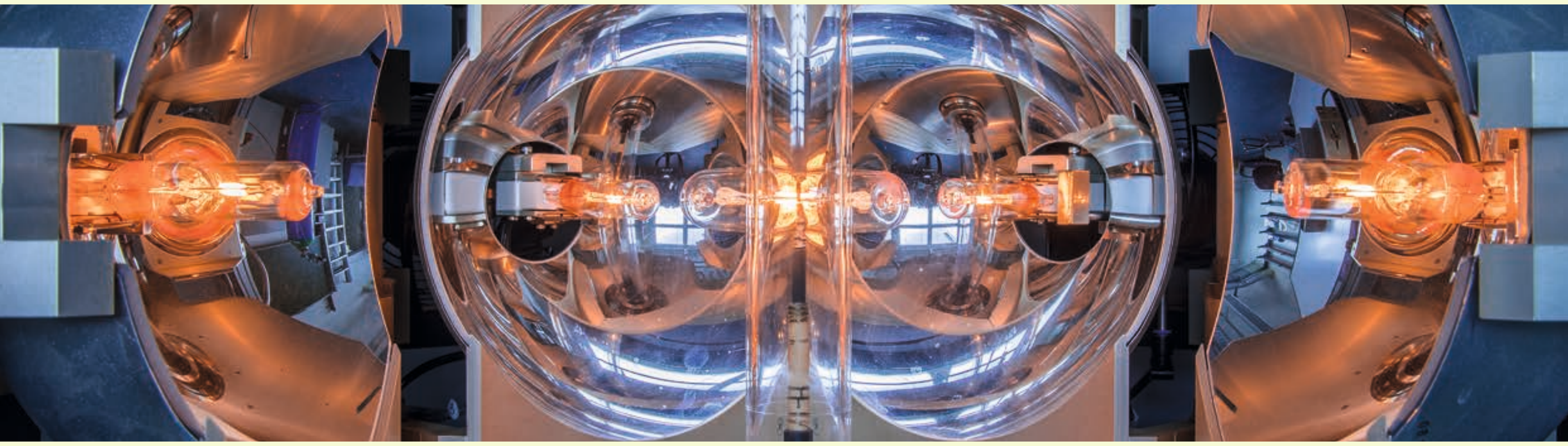
2020

Dr. Tristan Petit received an ERC Starting Grant from the European Research Council and with funding of 1.5 million euros over the next five years. The materials researcher is investigating a new class of materials for storing electrical energy, known as MXenes. They can store and release large amounts of electrical energy extremely quickly.

Jerome Deumer was awarded the Lise-Meitner Prize by Humboldt-Universität Berlin for his Master's thesis in which he investigated materials for energy storage.

Dr. Raphael Jay was awarded the Carl Ramsauer Prize of the German Physical Society in Berlin for his doctoral thesis. In his PhD work, he investigated ultrafast charge transfer dynamics in iron complexes.

Zone melting furnace in the crystal growth laboratory. © HZB/M. Setzpfandt



Dr. Max Grischek received the Erhard Höpfner Study Award and a stipend of 2,000 euros for his doctoral thesis in February 2020.

Dr. Danny Kojda received the 2020 Helmholtz Prize for the category “Precision Measurements in Applied Metrology”, Helmholtz Funds e. V. founded by the Physikalisch-Technische Bundesanstalt (PTB).

Dr. Martin Bluschke received the Springer Thesis Prize for his doctorate in January 2020 and the Ernst Eckhard Koch Prize in December 2020 awarded by the Friends of Helmholtz-Zentrum Berlin at the annual user meeting.

Tristan Petit in the experimental hall of BESSY II. © HZB/S. Steinbach

Steve Albrecht in the HySPRINT laboratory. © HZB/M. Setzpfandt

POSTER AND LECTURE AWARDS IN 2019/2020 WENT TO:

Alexander Arndt, Prince Saurabh Bassi, Jakob Bombsch, Joachim Breternitz, Raul Garcia Diez, Eike Gericke, Manuela Klaus, Maximilian Krause, Silvio Künstner, Frederike Lehmann, Laura Pardo-Perez, Götz Schuck, Andreas Siebert, Johannes Sutter, Peter Tillmann, Javier Villalobos, Zhenyu Wang, and Lifei Xi.

FACTS AND FIGURES FROM THE HZB

As of Dec. 31, 2020

1,172 EMPLOYEES

- **Proportion of women: 30 %**
- **Scientists: 532,** 117 of them women (22 %)
- **HZB science support staff: 238,** of which 62 are women (26.1 %)
- **Administrative, technical, and other staff of the HZB: 367,**
- of which 160 are women (43.6 %)
- **Trainees: 34,** thereof 12 women (35.3 %)

6 CORELABS

- Energy Materials in situ Laboratory Berlin (EMIL)
- X-Ray CoreLab
- CoreLab for Correlative Microscopy and Spectroscopy (CCMS)
- Hybrid Silicon Perovskite Research, Integration & Novel Technologies (HySPRINT)
- Competence Centre Thin-Film and Nanotechnology for Photovoltaics Berlin (PVcomB)
- CoreLab Quantum Materials

USERS FROM GERMANY, EUROPE, AND BEYOND

2019
2,370 external visits //1,317 users (double entries possible) from 30 nations
2020
939 external visits //625 users (double entries possible) from 20 nations

62

digital conferences and workshops were organised by HZB in 2020.

TEACHING

- Over 100 HZB scientists and scholars are **authorised to teach or have the right to award doctorates** at partner universities and are involved in teaching.
- **W3 professorships:** 11 in total, 3 of them women (27 %)
- **W2 professorships:** 16 in total, 5 of them women (31 %)

By way of comparison, the nationwide proportion of women professors in the subject group of mathematics and natural sciences is 19.3 %.

YOUNG **SCIENTISTS**

- 10 Young Investigator Groups at HZB
- PhD students:
  2019: 124, completed dissertations: 39
  2020: 143, completed dissertations: 25

3 GRADUATE SCHOOLS

MATSEC
Materials for Solar Energy Conversion, Dahlem Research School, Jan. 1, 2018 - Dec. 1, 2020

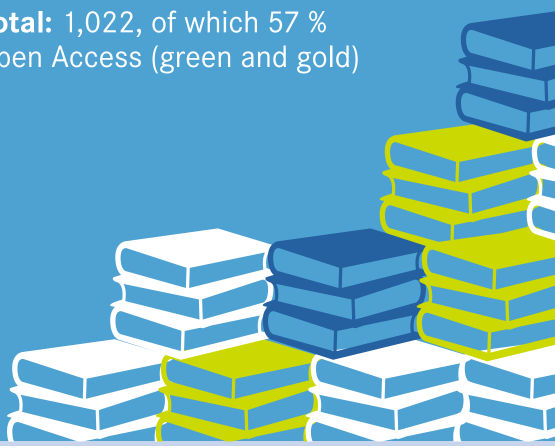
HYPERCELLS
Hybrid Perovskites Solar Cells, University of Potsdam, Technische Universität Berlin, Freie Universität Berlin, Humboldt Universität, Jan. 1, 2019 - Dec. 31, 2021

FIT
Future Information Technologies, Dahlem Research School, Jun 23, 2017- June 22, 2024

PUBLICATIONS

2020 total: 926, of which 61 % were Open Access (green and gold)

2019 total: 1,022, of which 57 % were Open Access (green and gold)



THE HZB BECOMES MORE SUSTAINABLE

The HZB has committed itself in its Code of Conduct not only to conducting sustainable research, but also to proactively protecting our natural resources. We set a course in 2019 for greater sustainability and have taken a big step forward. Here are the most important measures at a glance:

THE **ENVIRONMENTAL TEAM** OF THE HZB: A DRIVING FORCE

“We #AllForClimate!” - was the motto of the largest climate demonstration that took place in numerous cities around the world on September 20, 2019. Many employees from the HZB also took part in these rallies in their free time. In doing so, they wanted to show how important it is to them to fight the causes of climate change and to take action – now.
This strong personal commitment also leads many employees to actively search for resource-saving solutions in their work environment. At the end of 2018, around 20 employees joined together to form an environmental team that has since met every three months and has now grown to almost 50 participants. The environmental team discusses concrete proposals to improve the ecological balance of the research centre. Topics have included reducing heating energy and paper usage, sustainable campus design, and introducing fairtrade coffee products in the canteen.

IMPORTANT GOAL: **LESS FLYING**

In 2019, the environmental team drew up a proposal to significantly reduce business trips by air over the next two years - both domestic and international flights. The targets for reducing flights initiated by the environmental team were agreed with the HZB management in spring 2020. The tailwind for this should be great: for example, almost 150 employees from the HZB signed a voluntary commitment in 2019 to refrain from short-haul business flights of less than 1,000 kilometres (as part of the Scientists4Future campaign: “I won't do it for less than 1,000”). In addition, an Environment working group was established. It deals with the suggestions from the environmental team and brings them to the attention of the management. It also advises on how the measures can be implemented at the centre. This, too, shows the seriousness with which the HZB is proceeding in matters of climate protection and ecology.

100 PER CENT **GREEN ELECTRICITY** FOR RESEARCH

17,400 tonnes of CO_2 emissions have been eliminated by switching to green electricity.

The HZB consumes a large amount of electricity due to the operation of its large-scale facilities and laboratories. In the new tender for the electricity supplier, the HZB decided to purchase electricity exclusively from renewable sources beginning at the start of 2020. By switching to green electricity, 17,400 tonnes of CO_2 emissions per year can be eliminated. Independent of this, the HZB is exploring how to reduce its energy requirements. This is also a priority in the development of a design for the BESSY III successor source.

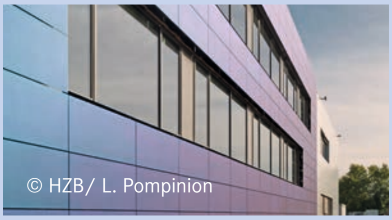
MORE BIODIVERSITY ON CAMPUS

Around 15 goats and sheep ensure that a lawn mower no longer has to be used on some near-natural areas. © HZB

“Sheep are grazing on the Lise-Meitner Campus in Wannsee”, the HZB proudly announced on its website in May 2019. This is not only insect- and bee-friendly, but also increases the biodiversity of the meadows - so that it will bloom and hum in the future!
On the other meadows, mowing has been considerable less frequent since 2019. Leaf vacuums are also prohibited and leaf blowers are only permitted in exceptional cases (on concrete). For the Adlershof Campus, the HZB commissioned a study to redesign the site in a nature-oriented manner. The first measures were implemented in 2020. “This will help us counteract insect mortality through natural, ecological design of the green spaces and make a positive contribution”, says Karin Haas, the HZB’s Sustainability Officer. In 2019, the HZB set course for important environmental and climate protection. But there is no time to rest. The HZB will have to intensify these efforts in the coming years in order to reduce carbon emissions even more farther. This is the only way to limit climate change.

FAÇADE WITH SOLAR MODULES AT THE HZB: A REAL-LIFE LAB

The Consulting Office for Building-Integrated Photovoltaics (BAIP) at the HZB offers advanced training in innovative façade solutions for professionals from architecture, planning, and construction. Now for the first time, a new HZB building has also been equipped with solar modules. This is the extension to the testing hall at BESSY II in Adlershof, in which components for accelerator physics are to be developed and tested. Solar modules now shimmer on the façade in an impressive matt-finish blue tone.



© HZB/ L. Pompinion

These are special CIGS thin-film modules produced in Germany that have been specially developed for integration with building envelopes. The solar façade not only covers part of the electricity demand, but is also a real laboratory itself: an HZB team will be monitoring the behaviour of the modules over the long term and under different outdoor conditions and evaluating the data.

A total of 360 modules have been mounted on the west, south and even on the north side of the outer shell. “It is a curtain wall”, explains Samira Aden, architect at BAIP/HZB, who is supervising the project. The modules are hung in front of the façade via a rail system so that a small air space is created between the module and the thermal insulation. “Through the additionally installed sensor technology, we will learn in the next few years how real weather conditions, fine dust, rain, and pollution affect the performance”, she explains.
“This photovoltaic project is something special”, emphasises Björn Rau, who heads BAIP. This will be the first time that a complete integrated photovoltaic system as been operated as a real laboratory. “In this project, we deliberately placed emphasis on integrating the design of the modules with the building envelope and selected CIGS technology as the material system – which the HZB has a great deal of expertise with”, adds Rau. Requests for data and experience are already coming in large numbers, including from abroad.

NEUTRON RESEARCH: THE INSTRUMENTS FROM BER II REMAIN INTACT AND AVAILABLE FOR RESEARCH

No neutrons have flown through the instruments at BER II since December 12, 2019. When the HZB Supervisory Board decided in summer 2013 to finally shut down BER II, the HZB management, the Supervisory Board, and the researchers agreed that the highly specialised neutron instruments should continue to be operated at other research facilities. After all, they contain a great deal of know-how. “For decades, BER II was well-known among experts for its development of unique instruments with highly specialised sample environments”, says Roland Steitz, who is coordinating the transfer of the neutron instruments.

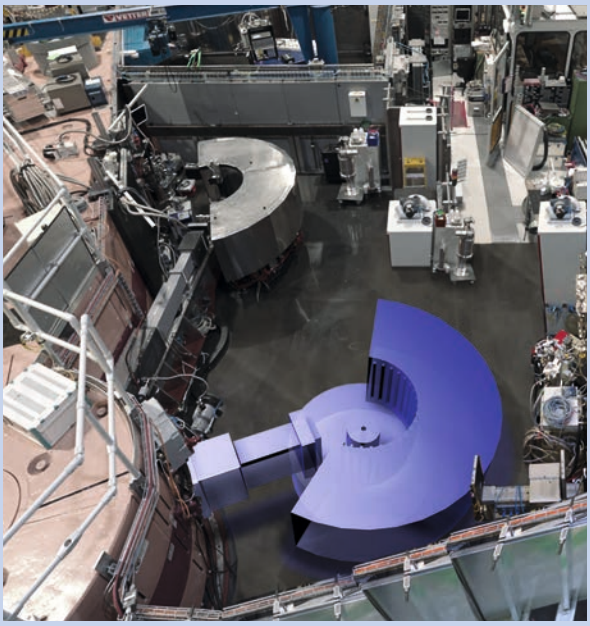
Neutron guide hall at BER II. © HZB/K. Fuchs

But how does someone find the right neutron source? As early as 2015, HZB contacted national and international research institutions that are currently building a neutron source or planning an expansion. 30 interested parties met for a workshop in Berlin in autumn 2015. “There we demonstrated the scientific performance of the instruments, but also talked about the technical requirements and the necessary preliminary planning needed to build and operate certain instruments”, **Roland Steitz** recalls.

“For me, it is also a matter of the heart that the neutron instruments can continue to be operated at other facilities.”

A few months after the workshop, the first letters of intent for the acquisition of neutron instruments started to arrive at the HZB. “We prioritised the written expressions of interest so that the neutron instruments would be transferred to facilities in Germany and Europe if possible, because the instruments were built with German funding. That is why the Supervisory Board approved every transfer”, says Steitz. For example, the Heinz Maier-Leibnitz Centre (MLZ) in Munich is taking over the FLEXX three-axis spectrometer, which will be called LaDiff in future and will offer Larmor diffraction.

In addition, the MLZ in future will also be home to the FIREPOD diffractometer. Both will move to Garching within the next four years.



Two powder diffractometers side by side: The high-resolution structural powder diffractometer SPODI (top) in the MLZ experiment hall will have FIREPOD as its neighbouring instrument in the future. © W. Schürmann / TUM, Illustration: R. Müller / FRM II, TUM

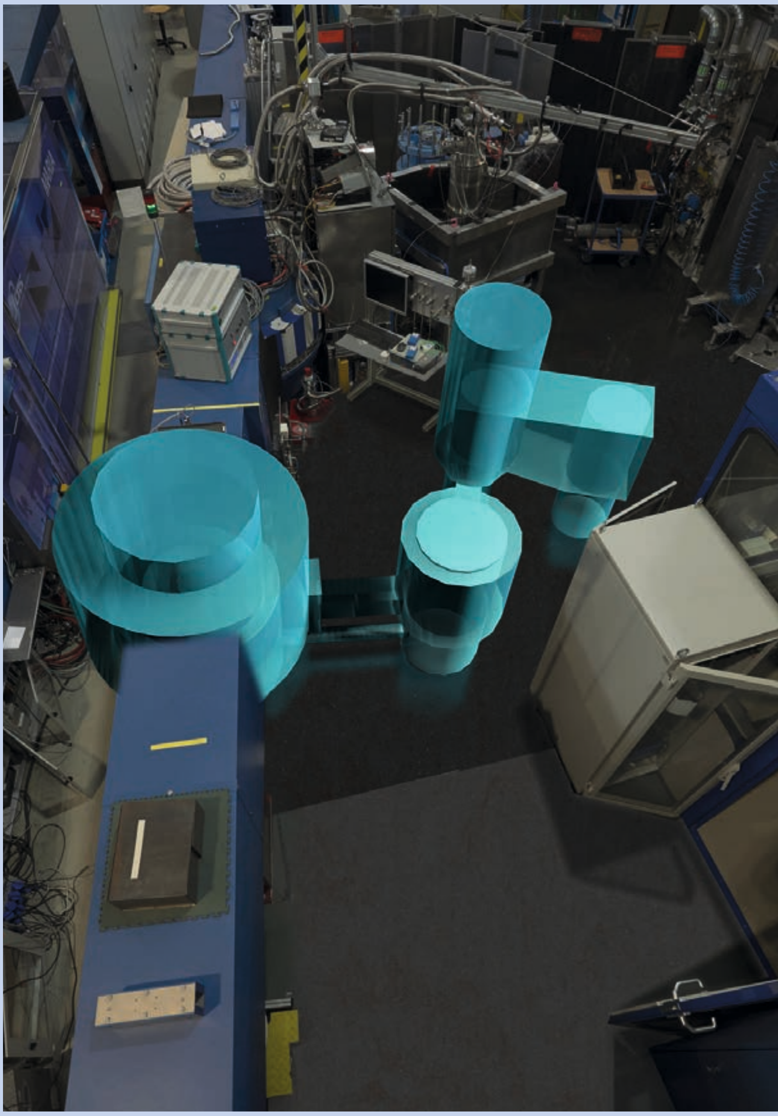
Experiment hall. © HZB / B. Ludewig

> "Both instruments were in great demand, with both our international scientific guests and our own teams gaining deep insights into complex material systems here and publishing their results in top journals."

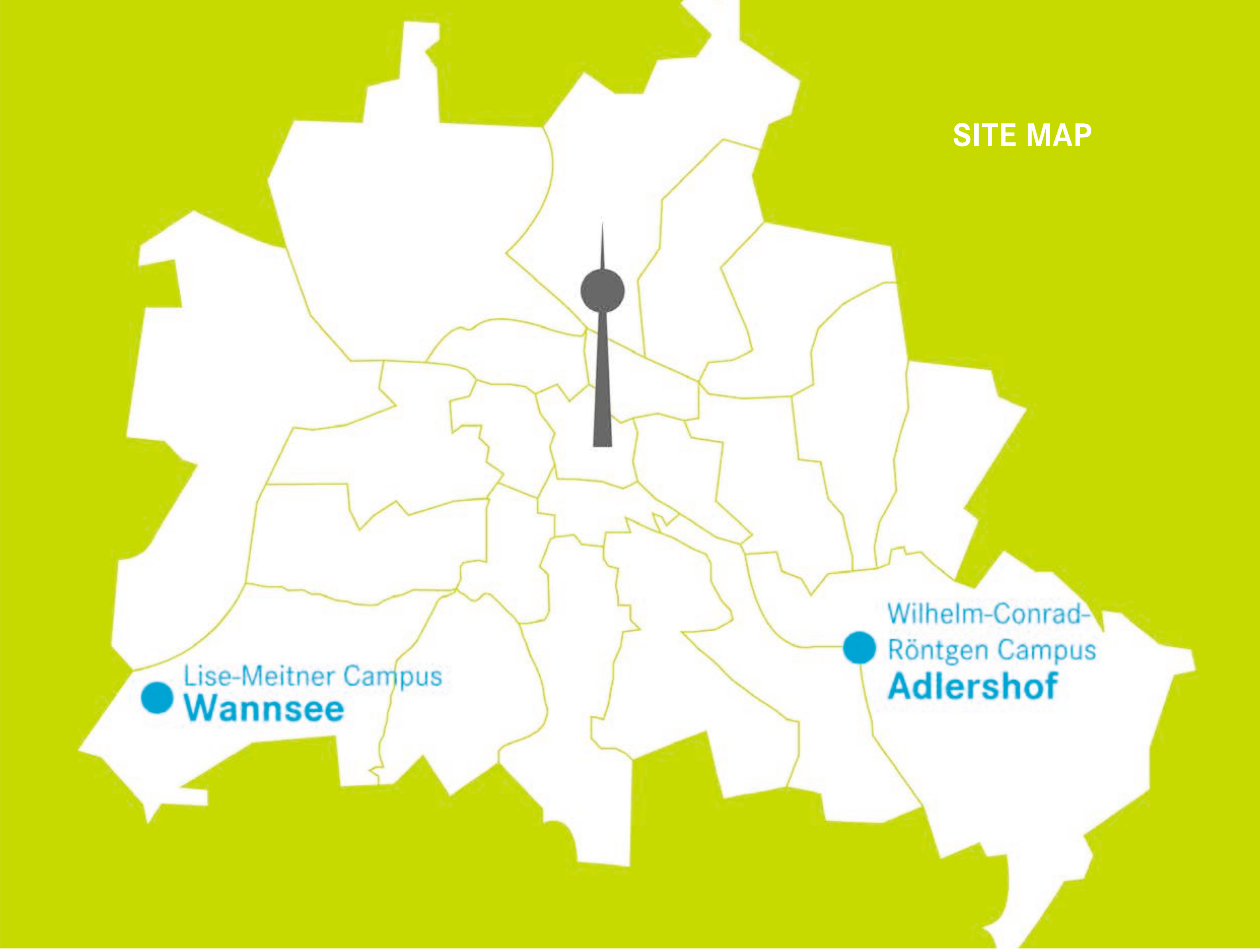
says **Jan Lüning**, Scientific Director of HZB. "We are therefore very pleased that these instruments at the MLZ will now continue to be available to the global neutron user community."

If no interested party was found from this circle, the HZB also negotiated takeovers by neutron sources from other parts of the world, such as for the BioRef neutron instrument, which is already in operation at the OPAL research reactor of the Australian Centre for Neutron Scattering southwest of Sydney. In the meantime, all the highly specialised instruments that were used at BER II either already have a new home or a concrete prospect for further use. Some instruments are so large and bulky that this work will take several months. But it is important for the dismantling of BER II that the experimental halls are empty. By the end of 2023, the last neutron instruments should therefore have been transferred – to new destinations where they can continue to serve the scientific search for knowledge.

Silvia Zerbe



The three-axis spectrometer LaDiff, which was still called FLEXX in Berlin, will be located in the neutron guide hall West of the FRM II in Munich next to the MIRA instrument. © Photo: W. Schürmann / TUM, Illustration: R. Müller / FRM II, TUM



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

Design & Layout: Heike Cords, Klaus Dieter Krön

Picture editors: Antonia Rötger, Heike Cords, Stefanie Kodalle

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Elbe Druckerei Wittenberg GmbH, Breitscheidstraße 17a, 06886 Lutherstadt Wittenberg
Tel.: +49 (0)3491 41 02 42, Fax: +49 (0)3491 41 02 40
E-mail: info@elbedruckerei.de, www.elbedruckerei.de

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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

Institute Silicon Photovoltaics

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

PVcomB

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