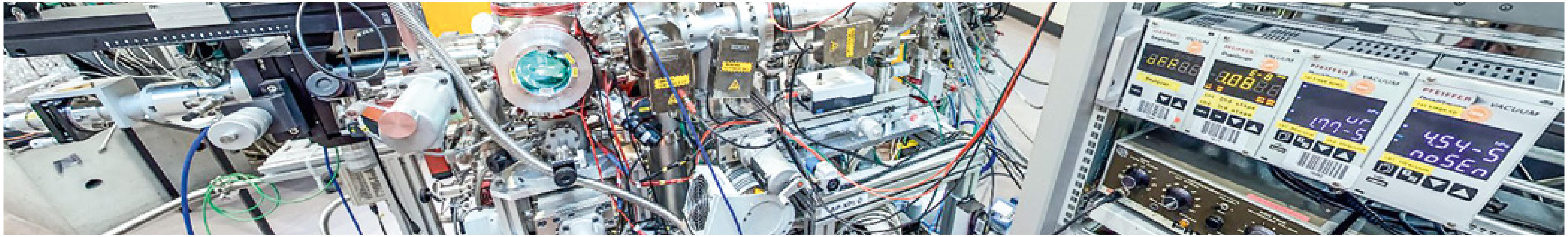
HZB Helmholtz Zentrum Berlin

HIGHLIGHTS 2021

Helmholtz-Zentrum Berlin
für Materialien und Energie

CONTENTS

Note: User experiments are marked with the symbol Ⓤ

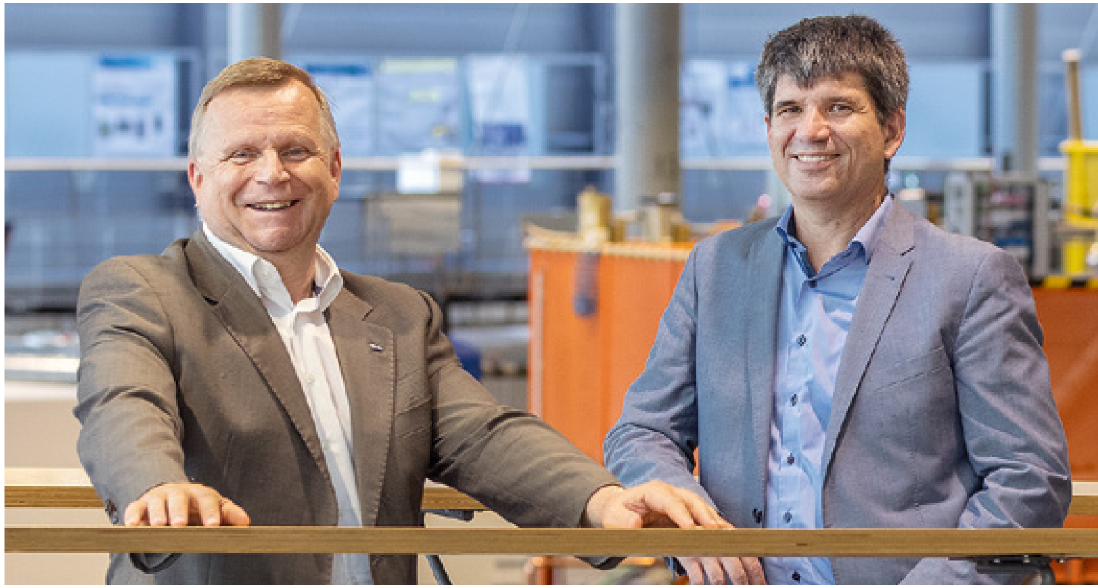


FOREWRD

Our staff, whether in research, technology or administration, have been highly productive even in times of pandemic. Last year, for example, we were able to launch a major project with financial support from the German Federal Ministry of Education and Research (BMBF): together with two Max Planck Institutes, we are setting up the Catlab research platform to develop new catalyst materials based on thin-film technologies. Among other things, such catalysts are needed to produce green hydrogen, but also to store it, transport it and process it further in the chemical industry. Green hydrogen is energy storage and raw material in one and will therefore be an important building block in the future energy system, which ought to be based on renewable, climate-neutral resources.

In this annual review, we have compiled a small selection from the 966 scientific publications that research groups from HZB and external user groups at HZB facilities have published. Divided into the three research areas of energy, information and matter, they provide an insight into the diversity of research at HZB and at our X-ray source BESSY II. It is certainly noticeable that research on perovskite-based solar cells is particularly well represented. We are proud of this, because several groups at HZB are now researching this exciting class of materials with very different focuses. The lively exchange between them is bearing fruit: in 2021, we once again achieved a new world record for the efficiency of a tandem cell made of silicon and perovskite; it was not until mid-2022 that the last record value of 29.8 percent was topped by a Swiss team. The race for ever higher efficiencies continues.

At the same time, HZB teams are also developing manufacturing processes that are compatible with industry, increasing stability or looking for even more environmentally friendly alternatives. To make the rapidly growing knowledge clearly accessible, a group at HZB, together with more than 30 international partner institutions, has designed a “wiki” with results from perovskite research.



Thomas Frederking (left), Commercial Director, and Professor Bernd Rech, Scientfic Director of Helmholtz-Zentrum Berlin für Materialien und Energie. © P. Dera/HZB

Accelerator physics remains an important field of activity at HZB. We are working on the design of new components for an upcoming upgrade of BESSY II and are constantly developing the instruments and measurement methods. Currently, the X-ray source BESSY II is a strong attractor for measurement guests from Germany and abroad. To ensure that this remains the case and that we can continue to offer state-of-the-art or even unique measuring stations in the future, we are not resting on our laurels, but planning for the future.

Thomas Frederking
Commercial Director

Bernd Rech
Scientific Director

"I AM ABSOLUTELY THRILLED AT HOW INTERNATIONAL WE HAVE BECOME"

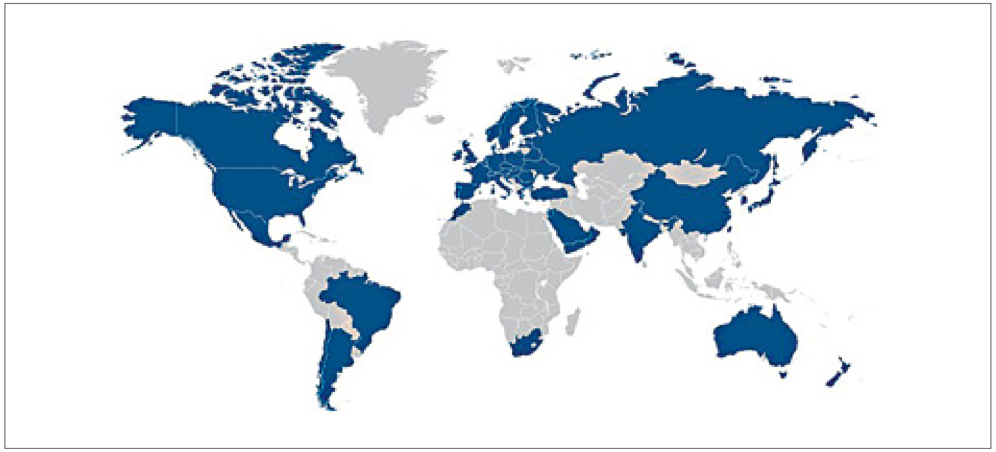
For 75 years, synchrotron radiation sources have been indispensable for gaining knowledge. **Antje Vollmer**, who heads the User Coordination department at BESSY II at HZB, talks about international networking and how she can already tell from the research proposals which social problems are particularly pressing at the moment.

Dr. Vollmer, you worked at BESSY for the first time in 1994 ...

Yes, that was while doing my PhD thesis. I was given measurement time there already in the first week. And a lot has changed since then.

Tell me about it!

The use of synchrotron radiation sources has become much broader. At BESSY I, 90 percent of the projects were for physics. Now, at BESSY II, 45 percent of the projects are for physics, while the rest are mainly for chemistry, biology, biochemistry, medicine and archaeology.



Researchers from many countries around the world submit proposals for measurement time at BESSY II.
© J. Politt/HZB

Does this also mean that the scientific questions that can be explored using synchrotron radiation have changed?

Quite distinctly. Today, there is a more pronounced motivation to derive practical, societal benefits from scientific findings. This is especially clear when it comes to major problems like the coronavirus pandemic: in its first year, COVID-19 papers based on work done at a synchrotron were being published at an average rate of one every five days – including, among other places, here at BESSY II.

When the pandemic started, did you systematically make measurement time at BESSY II available for COVID research?

We immediately fast tracked it at all experimental stations. Studies included not only protein structures, which is a long-standing branch of research here, but also aerosol distribution in the air, for example. During that phase, by the way, we set a new record: it took only three days from application to measurement – the typical lead time is half a year.

Outside of Corona times, are the socially burning issues also reflected in the applications you get on the table?

We actually do see which issues are particularly relevant and even exciting at the moment. For example, graphene becomes a hot topic and all of a sudden the number of applications skyrockets, until at some point it drops again. A cycle like that lasts about ten years. At the moment, energy research is high on the agenda, and I am sure it will keep us busy for much, much longer than the usual ten years. But of course, within such a large topic area, you also get shifts in focus. In the beginning, it was mainly on solar cells; currently, focus is on all aspects of energy storage, like hydrogen, battery research, electromobility or synthetic fuels – these are all topics that we would not have found here 20 years ago.

What about the user groups? Are they also becoming more diverse?

Oh yes! I recently looked at the 30-year-old user data, and in one year, for example, we had 114 German user groups, two Austrian groups and one Australian group. Today, international users make up almost half. I really am thrilled at see how international we have become here.

It sounds like there is more to it, though?

Unfortunately, the fact is that most of our user community comes from the northern hemisphere. Occasionally, we have someone from North or South Africa, but we have still never had any user groups from Central Africa.

Why would that be?

I can imagine it has to do with the societal structures. In Africa, there are 169 scientists per million inhabitants. In Europe, there are twenty times that. When I think of it, it reminds me of the European Union's TNA programme, which used to exist …

… TNA stands for trans-national access …

… and the EU would bear the costs if scientists crossed a national border for an experiment. It was supposed to promote maximum mobility in Europe. Back then, I trav-elled all over Europe and promoted BESSY II to researchers – in Romania, Bulgaria, Croatia, Portugal and many other countries. And everywhere I met with reservation. In Eastern Europe, the widespread attitude was that staying in Germany was unaffordable anyway – despite all costs including travel being covered. And in Southern Europe, the reservation was more along the lines that "we in the North" were a tight-knit club and would not take applications from the South seriously anyway.

"Today, international users account for almost half of all researchers who receive measurement time at BESSY II."

The term "science diplomacy" has come into use for what you are talking about now.

And a certain particle accelerator is a prime example of this: CERN, which was built after the war, was so large that it was too big for any one of the participating countries alone, and they could only manage it all together. A more recent example is the SESAME synchrotron in Jordan. It, too, is designed to bring together researchers from across the region, including Israel. That really is groundbreaking, even if the reality of it is not always so easy.

SESAME wants to become a synchrotron for African researchers as well …

And that brings me back to my observation that there are only few African scientists working here in Berlin. By the way, I had a moment of sudden insight at a conference of the Humboldt Foundation. We had colleagues from Kenya, Bangladesh and Myanmar there, working, for example, on water splitting for sustainable energy. For many of them, it was their first time at an international conference because they would normally not have been able to afford it. But because it was a virtual format due to COVID-19, they could all be there together. That's when it really hit me: often, we were simply excluding the whole of Africa from the brain circulation process – as we call it here at Helmholtz – just because many people over there couldn't travel for financial reasons. To get everyone involved, we should definitely make such meetings hybrid in the future, so that people can at least join in online. That, already, would be a significant step.

Short biography

Dr Antje Vollmer heads the User Coordination department at the X-ray source BESSY II and has been the spokesperson for this facility since 2021. As early as 2003, Vollmer, who holds a doctorate in chemistry, set up a measuring station at BESSY II and headed it for eight years before switching to user coordination ten years ago. She attaches great importance to the societal benefits of research at X-ray sources.

© D. Ausserhofer/HZB

We conducted the previous part of this interview in January 2022. What would you add today, half a year later, in the face of the war on Ukraine?
The Russian State's war of aggression against Ukraine shocks us all and shows how developments that we in Europe thought no longer possible are overrunning us. This war demands a clear stance against aggression and has led to clear, visible measures such as the immediate cessation of all cooperation with Russian institutions. It is the responsibility of the scientific community to take a clear stand against the behaviour of the Russian State – and that is what we at HZB have done. I would like to emphasize that this is about the Russian and Belarussian governments, not about the nationality of the colleagues. Our solidarity is with the Ukrainians, but also with the critical Russian scientists who are courageously taking a stand against the war. One thing that I firmly believe in was said well by the President of the German Physical Society: "We will not be shaken in our belief in the unifying effect of science!"

Interview: Kilian Kirchgessner

HZB HAS BEEN CERTIFIED FOR ITS STRATEGIES IN DEALING WITH DIVERSITY

The Helmholtz-Zentrum Berlin is the first non-university research institution to have undergone the Stifterverband's diversity audit "Shaping Diversity". The certification attests to the HZB's **opportunity-oriented concepts and measures** for diverse groups of people.

Dr Volker Meyer-Guckel (left), Deputy Secretary General of the Stifterverband, presented Dr Jennifer Schevardo, HZB Project Manager Diversity Audit, and Professor Jan Lüning, then Spokesperson for the HZB Management Board, with the "Shaping Diversity" certificate. © HZB

Regardless of whether employees come from abroad, have a migration background or work part-time, regardless of their age, gender or ideology – all employees should be able to participate equally in everyday work with their abilities. To ensure this, the HZB went through an 18-month process. In the process, the existing concepts to promote diversity were expanded and corresponding measures were implemented. These concern both organisational structures and personnel management. Services for employees and diversity-sensitive communication are also part of the diversity strategy.

"The diversity audit has given us important impetus and pushed forward issues that we have been dealing with as an organisation for a long time," says Thomas Frederking, Commercial Director of HZB. "We have updated our Code of Conduct, organised selection and recruitment processes in a more diversity-sensitive way and are currently revising the processes for conflict management. We have also taken a close look at our work and leadership culture and will establish corresponding guidelines. Many HZB employees contributed ideas during the diversity audit, which we are particularly pleased about."

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CATLAB – STARTING SIGNAL FOR A NEW GENERATION OF CATALYSTS

The **CatLab catalysis centre**, a joint research platform of HZB and the Max Planck Society, went into operation in summer 2021. The goal is to efficiently produce and process **green hydrogen** with the help of new catalysts.

Opening ceremony of CatLab (f.l.t.r.): Professor Bernd Rech, Scientific Director of HZB, Dr Stefan Kaufmann, Member of the Bundestag and Innovation Officer for Green Hydrogen, and Professor Robert Schlögl, Scientific Director of FHI and MPI CEC. © M. Setzpfandt/HZB

Hydrogen is a key building block for the energy transition to be successful. However, for this versatile energy medium to really be sustainable, it must be produced using renewable energy. At the same time, new sustainable technologies are needed for processing green hydrogen into industrial feedstock. The processes required for this have something in common: they cannot be carried out using conventional catalysts – a new generation of catalytic processing is required. This is precisely the core mission of CatLab. The researchers at the catalysis centre aim not only to develop novel, tailor-made catalysts using thin-film technologies and readily available chemical elements and compounds, but also to redesign the necessary catalysis equipment. This effort should produce the innovative breakthroughs needed to build a sustainable hydrogen economy.

To achieve this, HZB and the two Max Planck institutes, the Fritz Haber Institute (FHI) and Institute for Chemical Energy Conversion (MPI CEC), are pooling their expertise and establishing the Catalysis Centre together with university and industrial partners. CatLab is intended to build a bridge between basic research and industry through funding of around 58 million euros provided by the German Federal Ministry of Education and Research (BMBF)as part of the National Hydrogen Strategy. The five-year development project involves more than 100 million euros in total.

Professor Robert Schlögl, Scientific Director of FHI and MPI CEC, emphasized the timeliness: “With our in-depth understanding of catalysts and material synthesis at FHI and CEC, HZB‘s expertise in thin-film technologies, and the capability of conducting tightly integrated research on site with the HZB BESSY II synchrotron, this constellation gives us a unique opportunity to advance the new field very quickly. CatLab will take our ability to design high-performance catalysts to a new dimension. We will be able to rapidly translate basic research findings into a much-needed technology push.”

Professor Bernd Rech, Scientific Director of HZB, said: “We will contribute a lot of know-how we have developed in researching thin films for solar cells at HZB. And BESSY II has already contributed essential insights into the understanding of catalysts. We have been working with catalysis researchers from all over the world for many years. All of this helps us to achieve critical mass with the collaboration we have now launched through CatLab. With strong involvement from Humboldt Universität zu Berlin and the Berlin Cluster of Excellence UniSysCat, as well as early participation of partners from industry, we will contribute significantly to the design of a future sustainable energy system.”

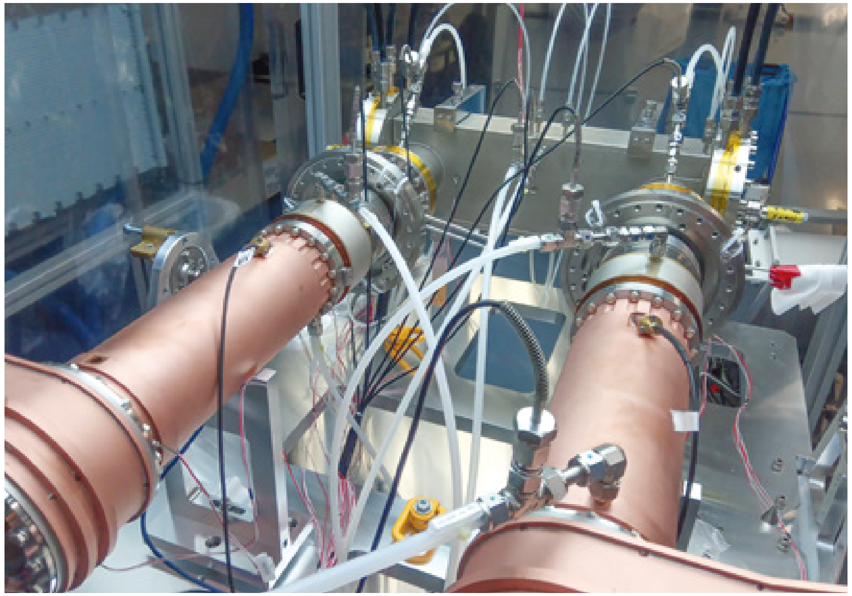
In close cooperation with Humboldt Universität (HU), the newly completed laboratories in HU‘s IRIS research building in Adlershof provide an optimal setting for the launch of CatLab. At the same time, the catalysis research centre will be expanded in several construction phases over the long term.

BERLINPRO – HF-COUPLERS PROVE RESILIENT

At the HZB site in Adlershof, researchers have built a prototype of a **linear accelerator with energy recovery (bERLinPro)**. They were able to take another important step in the development of the globally unique key components needed for the facility before the project was completed at the end of 2021.

In synchrotron light sources, an electron accelerator brings electron bunches to almost the speed of light so that they can emit the special "synchrotron light". The electron bunches get their enormous energy and their special shape from a standing electromagnetic alternating field in so-called cavities. With high electron currents, as required in the bERLinPro project, the power needed for the stable excitation of this high-frequency alternating field is enormous. The coupling of this high power is achieved with special antennas, so-called couplers, and is considered both a great scientific and a technical challenge.

These couplers should supply the cavities with 230 kilowatt in continuous operation at 1.3 gigahertz (GHz). The connection between the ultra-high vacuum of the cavities and the high-frequency transmission link must be guaranteed, both at liquid helium temperature (-269 degrees Celsius or 4 Kelvin) and at room temperature. In addition, clean room conditions must be maintained and particles down to the micrometre range must be removed. The power is to be transferred to the cavity by two couplers each, in order to reduce the individual load and to improve the stability of the electron trajectory in the accelerator.



For the measurement campaign, two couplers were mounted in a horizontal test position under a local clean room tent. © A. Neumann/HZB

The team led by Axel Neumann from the HZB Institute SRF (Superconducting Radio Frequency Technologies) has been able to show that this goal is realistic. To do so, they modified the design of the high-performance couplers of a group from the National Research Centre for High Energy Physics in Japan (KEK). The measurements started with low power, which was gradually increased up to 45 kW. Initially, only short pulses were transmitted from the couplers to the cavity at longer intervals, here even up to powers of 100 kW. Then the intervals between the power pulses became shorter and shorter up to continuous operation.

The heat development was 0.25 Kelvin per kilowatt of power. At a final power of 120 kW, the material would heat up by about 30 degrees Kelvin. This is good news, because such amounts of heat are technically dissipatable through the planned cooling. „With the original Japanese design, the heat generation was higher by a factor of four than with our adapted form," explains Neumann. "We initially limited the measurements to power levels below 45 kW. Only when all couplers have been successfully tested at these powers will the next steps come. However, we are now very optimistic. If you extrapolate the figures, the coupler should indeed manage 120 kW in continuous operation without any problems," says Jens Knobloch, who heads the HZB Institute SRF Science and Technology. *arö*

HZB USES ELECTRICITY-PRODUCING FACADE WALL AS REAL LABORATORY

In the presence of the State Secretary for Economic Affairs, Energy and Operations of the State of Berlin, Christian Rickerts, the HZB officially commissioned the **solar facade of a new research building** in september 2021. What makes it so special is that the elegant façade not only generates up to 50 kilowatts of electricity. It also provides important insights into the behaviour of the solar modules under different weather conditions.

Solar energy is considered one of the most promising renewable energies. More and more houses have a photovoltaics on the roof and large open-space systems are increasingly being seen. But solar modules can also be integrated in more diverse ways, for example in building facades. Through the solar activation of the entire building envelope, photovoltaics becomes a building element and turns buildings into electricity generators. Moreover, the solar modules can also be integrated in a visually appealing way. For two years now, the HZB-based consulting office for building-integrated Photovoltaics (BAIP) has been providing advice on precisely this topic.

Since september 2021 the HZB itself is doing the practical test. “For the first time, a complete building with a facade-integrated photovoltaic system is being operated as a real laboratory. The extensive measurement technology enables new insights into the real behaviour of solar modules in a facade in different seasons and weather conditions, over a long period of time,” says Björn Rau, who heads the BAIP office at HZB.

The Real Lab consists of 360 thin-film solar modules made of copper indium gallium diselenide (CIGS) installed on three sides of the facade. The output of each module is approximately 135 watts. The peak power of the entire façade is just under 50 kilowatts. Among other things, 72 temperature, ten irradiation and four wind sensors were installed as additional sensor technology. The facade is used for long-term investigation of PV yields as a function of environmental factors (pollution), weather conditions (sun, wind, reflection) and compass directions. This enables a comparison between real data and simulation values of yield forecasts.

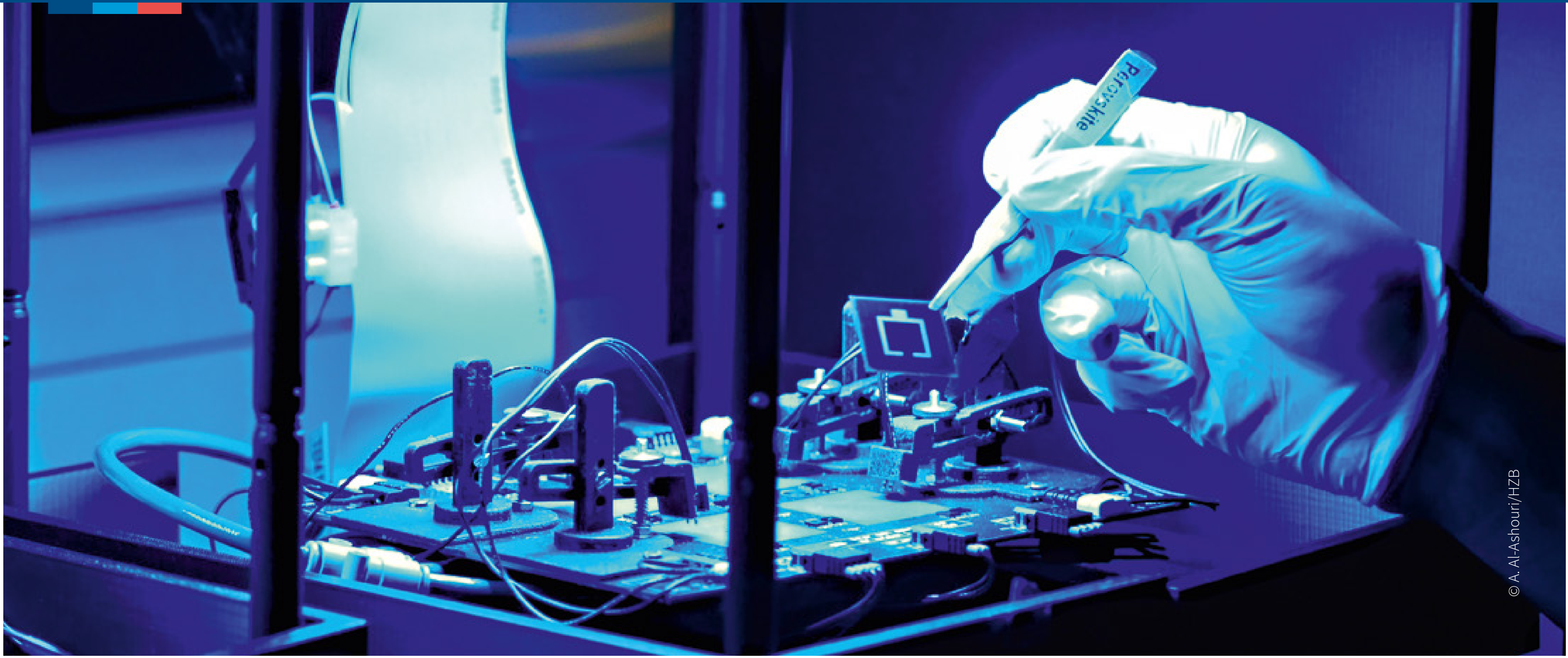
A special feature is the concealed suspension. It enables a frameless design without additional edging at the edge of the module. This makes it possible to combine the modules ideally with the metal curtain wall of the building. Björn Rau emphasises: “We also deliberately placed value on the design integration of the modules into the building envelope and, with CIGS technology, selected the material system about which there is a very great deal of expertise at HZB.” Many research groups at HZB work with CIGS thin films, from materials research to the development of building elements.

Professor Bernd Rech (left) and Christian Rickerts pressed the symbolic red button to start the Real Lab in Berlin-Adlershof. © M. Setzpfandt/HZB

The facade serves as a real laboratory for photovoltaics research, but something completely different happens inside the building: here, researchers develop and build worldwide unique components for BESSY II and other synchrotrons. The building houses a clean room, various laboratories and assembly stations for HZB’s internationally renowned accelerator research. *red.*

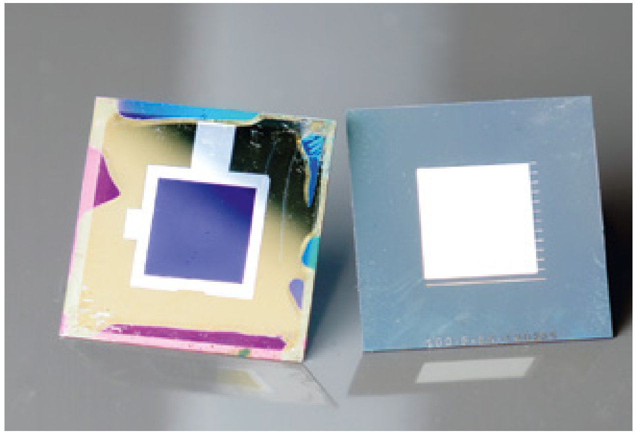
HIGHLIGHTS FROM OUR RESEARCH – ENERGY

HZB has a leading international position in photovoltaic research, but also makes important contributions in the field of energy storage. For example, scientists are working in battery research and on the development of catalytically active materials, for example to produce green hydrogen via electrolysis. **There is a more detailed text on almost every news item in the HZB Newsroom. Click on this symbol: ➲ There you can also search for data and keywords.**



WORLD RECORD FOR TANDEM SOLAR CELLS

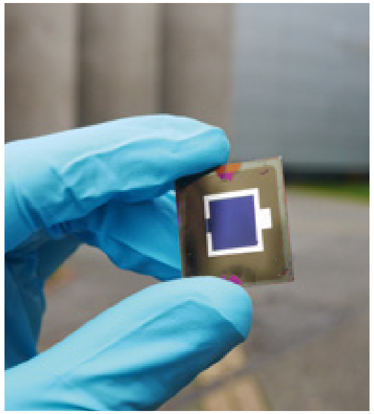
Three HZB teams led by Christiane Becker, Bernd Stannowski and Steve Albrecht have jointly succeeded in increasing the efficiency of completely in-house produced perovskite silicon tandem solar cells to a new record value of 29.8 percent*. The value was officially certified and recorded in the charts of the National Renewable Energy Laboratory. This brings the 30 percent mark within reach. At HZB, several groups of scientists have been working intensively since 2015 on both the perovskite semiconductors and silicon technologies and the combination of both into innovative tandem solar cells. "An efficiency of 30 percent is like a psychological limit for this fascinating new technology. It could revolutionise the photovoltaic industry in the near future," explains Steve Albrecht, who studies perovskite thin films in the HySPRINT Innvovation Lab at HZB.



The perovskite silicon tandem cell is based on two innovations: A nanotextured front side (left) and a back side with dielectric reflector. © A. Cruz/HZB

Nanotextured silicon

For the tandem solar cell, the focus was on the optical improvement of the silicon heterojunction bottom cell. For the new work, Philipp Tockhorn (Albrecht group) and doctoral student Johannes Sutter (Becker group) investigated how nanostructures at different interfaces affect the performance of a tandem solar cell consisting of a perovskite solar cell on a silicon solar cell. First, they used a computer simulation to calculate the photocurrent density in the perovskite and silicon subcells for different geometries with and without nanotextures. Then they produced perovskite silicon tandem solar cells with different textures: "Even nanotexturing on one side improves light absorption and enables a higher short-circuit current compared to a flat reference," says Sutter. And Tockhorn adds: "Remarkably, the nanotextures also lead to a slight improvement in the electronic quality of the tandem solar cell and to better film formation of the perovskite layers." Improvements have also been made to the back of the cell, which is designed to reflect infrared light back into the silicon absorber. "By using a dielectric reflector, we were able to use this part of the sunlight more efficiently, resulting in a higher photocurrent," says Alexandros Cruz Bournazou, postdoc in Stannowski's group.



The world record cell (here in front of the electron storage ring BESSY II) has an area of about one square centimetre, which is usual for research purposes, and achieves an efficiency of 29.8 percent. © A. Al-Ashouri/HZB

Further improvements are expected

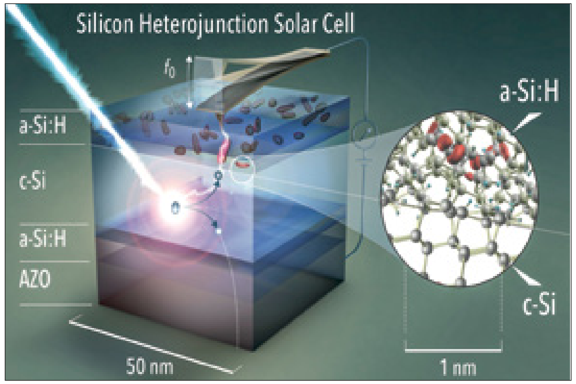
The results point the way for further improvements. Because the simulations suggest that the performance could be increased even further by nanostructuring the absorber layers on both sides. The researchers are convinced that an efficiency of significantly more than 30 percent could be achieved. The race for the best tandem solar cell remains exciting. *arö*

** This world record value was valid until the summer of 2022. In the meantime, it is over 30 percent (EPFL in Lausanne).*

Publication on the previous "word record cell":

Science (2020): Monolithic perovskite/silicon tandem solar cell with >29% efficiency by enhanced hole extraction. A. Al-Ashouri, E. Köhnen, A. Magomedov, H. Hempel, P. Caprioglio, J.A. Márquez, A. Belen Morales Vilches, E. Kasparavicius, J.A. Smith, N. Phung, D. Menzel, M. Grischek, L. Kegelmann, D. Skroblin, C. Gollwitzer, T. Malinauskas, M. Jošt, G. Matič, B. Rech, R. Schlatmann, M. Topič, L. Korte, A. Abate, B. Stannowski, D. Neher, M. Stoltefoht, T. Unold, V. Getautis, and S. Albrecht. **DOI: 10.1126/science.abd4016**

SOLAR CELLS: LOSSES MADE VISIBLE ON THE NANOSCALE



A conductive AFM tip is used to scan the sample surface of an a-Si:H/c-Si interface under ultra-high vacuum on the nm scale. This reveals the transport channels of the charge carriers via defects in the a-Si:H (red states in the magnified section). © M. Künsting/HZB

Solar cells made of crystalline silicon achieve peak efficiencies, especially in combination with selective contacts made of amorphous silicon (a-Si:H). However, their efficiency is limited by losses in these contact layers. Now a team at HZB and the University of Utah, USA, has experimentally shown how such contact layers generate loss currents on the nanometre scale and what their physical origin is. Using a conductive atomic force microscope, they scanned the solar cell surfaces in ultra-high vacuum and detected tiny, nanometre-sized channels for the detrimental dark currents, which are due to disorder in the a-Si:H layer. The results indicate that a short-term current blockade is present, which is caused by local charge that is trapped in neighbouring defects which changes the energetic positioning of the tunnelling states. This trapped charge can also cause the local photovoltage at a current channel to rise to above one volt, which is far above what one would be able to use with a macroscopic contact. "At this transition from the nano to the macro world we find the exciting physics of heterojunctions and the key on how to further improve the efficiency of silicon solar cells in an even more targeted way," says Bernd Stannowski, who is responsible for the development of industrial silicon heterojunction solar cells at HZB.

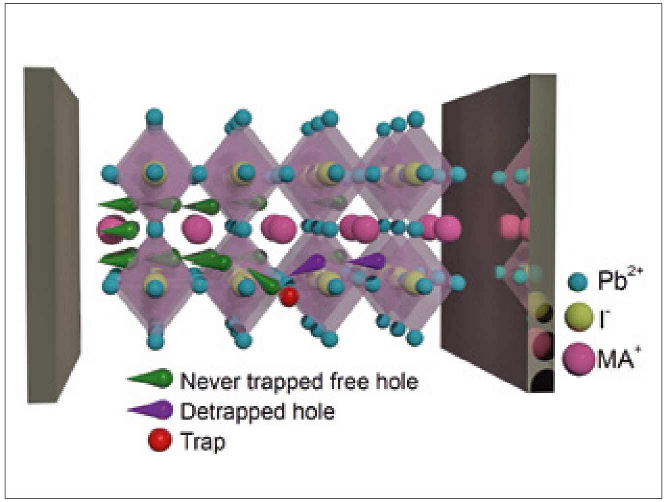
arö

ACS Applied Nano Materials (2021): Imaging of Bandtail States in Silicon Heterojunction Solar Cells: Nanoscopic Current Effects on Photovoltaics. M. Y. Teferi, H. Malissa, A. Belen Morales-Vilches, C. T. Trinh, L. Korte, B. Stannowski, C. C. Williams, C. Boehme, and K. Lips. **DOI: 10.1021/acsanm.0c02704**

DEFECTS TRAP CHARGE CARRIERS IN PEROVSKITE SOLAR CELLS – AND RELEASE THEM AGAIN

An international team of HZB and Charles University Prague has investigated how charge carriers in so called MAPI-perovskite semiconductors interact with different defects. They show that a large proportion of defects quickly releases trapped charge carriers. The measurement results allow the reliable differentiation between electron and hole transport and the determination of their most important parameters: Mobilities, lifetimes and diffusion lengths. "This work thus provides answers to questions that have been discussed for a long time in the field of perovskite solar cells," says Artem Musiienko, first author of the publication and postdoc at HZB.

An important finding: a large proportion of the defects release the captured charge carriers again after a short time. "This may partly explain these particularly high efficiencies of the MAPI perovskites," says Musiienko. These results pave the way to optimise MAPI perovskites in terms of defect concentration, combining high efficiencies with good stability.



Five different types of defects in MAPI-perovskites were examined and characterised. The result: a large proportion of defects is not trapping the charge carriers for long. © HZB

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Advanced Functional Materials (2021): Defects in Hybrid Perovskites: The Secret of Efficient Charge Transport. A. Musiienko, D. R. Ceratti, J. Pipek, M. Brynza, H. Elhadidy, E. Belas, M. Betušiak, G. Delport, and P. Praus. **DOI: 10.1002/adfm.202104467**

LEAD-FREE PEROVSKITE SOLAR CELLS – HOW FLUORIDE ADDITIVES IMPROVE QUALITY

Lead halide perovskite solar cells promise very high efficiencies at low manufacturing costs. However, the toxicity of lead poses serious environmental concerns, proving the need for lead-free alternatives. Tin is currently considered the best choice, but faces challenges regarding its oxidation and uncontrolled crystallization that restrains the respective solar cells in their production, performance and stability. One of the most common strategies to obtain good quality tin-based perovskite thin-films involves the use of tin fluoride (SnF_2) as an additive in the solution-based process. The improved optoelectronic and morphological properties of SnF_2-containing films have been thoroughly characterised in literature, although the role of this additive remained underexplored.

Intercalation into the perovskite structure observed

A team led by Antonio Abate has for the first time elucidated the important chemical role of SnF_2 inside the perovskite solution that is responsible for these improvements. The key lies in the chemical behaviour of fluoride anions. Tin easily oxidises from Sn(II) to Sn(IV), generating defects in the semiconductor film. Data from nuclear magnetic resonance (NMR) analyses now showed that the fluoride anion from SnF_2 has a strong affinity for Sn(IV) and forms the compound SnF_4. Using hard X-ray photoelectron spectroscopy at BESSY II, the team was able to demonstrate that SnF_4 shows a lower tendency to be entrapped in the perovskite structure compared to SnF_4, resulting in less Sn(IV) content in the film. Finally, small-angle X-ray scattering measurements at BESSY II revealed that the fluoride appears to positively affect the nucleation process in the precursor solution, which improves crystallisation.

More homogenous crystal growth

"To put it simply, fluoride anions trap oxidized Sn(IV) in the solution, as SnF_4. The lower affinity of this material to perovskite-like species prevents its inclusion in the perovskite film," says Jorge Pascual, a postdoc from Abate's group working on tin halide perovskites. "In addition, fluoride improves the colloid stability of tin halide perovskite precursor solutions, precursor subunits creating a more uniformly distributed oriented attachment, resulting in a more homogeneous crystal growth," explains Marion Flatken, who carried out the research as part of her PhD in the same team.

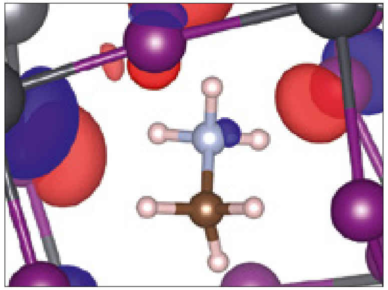
These results come at the right time. Based on this study, it might be possible to explore other promising additives that further improve the properties of lead-free perovskite solar cells. *arö*

Fluoride additives increase the quality of the perovskite layer. At BESSY II a team has now explored the chemistry in detail.

Angewandte Chemie, international Edition (2021): Fluoride Chemistry in Tin Halide Perovskites. Jorge Pascual, Marion Flatken, Roberto Félix, Guixiang Li, Silver-Hamill Turren-Cruz, Mahmoud H. Aldamasy, Claudia Hartmann, Meng Li, Diego Di Girolamo, Giuseppe Nasti, Elif Hüsam, Regan G. Wilks, André Dallmann, Marcus Bär, Armin Hoell, Antonio Abate. **DOI: 10.1002/anie.202107599**

PEROVSKITE SOLAR CELLS: HYDROGEN BONDS MEASURED

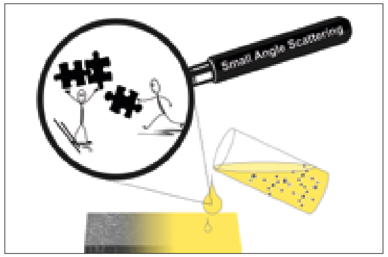
Based on X-ray measurements of methylammonium perovskite semiconductors, an HZB team has shown the role played by hydrogen bonds in these materials. In addition, the research group demonstrated that radiation damage by soft X-rays to this sensitive class of materials occurs even faster than often expected. A reason why it is also associated with instability. Both results provide important information for perovskites materials research for solar cells. *arö*



Orbital hybridization between organic and inorganic components of MAPI perovskite in ground-state geometry. © HZB

Journal of Physical Chemistry Letters (2021): Dynamic Effects and Hydrogen Bonding in Mixed-Halide Perovskite Solar Cell Absorbers. R. G. Wilks, A. Erbing, G. Sadoughi, D. E. Starr, E. Handick, F. Meyer, A. Benkert, M. Iannuzzi, D. Hauschild, W. Yang, M. Blum, L. Weinhardt, C. Heske, H. J. Snaith, M. Odelius, and M. Bär. **DOI: 10.1021/acs.jpclett.1c00745**

INSIGHTS INTO EARLY STAGES OF STRUCTURE FORMATION



Perovskite solar cells have been explored by using small-angle scattering. © M. Flatken/HZB

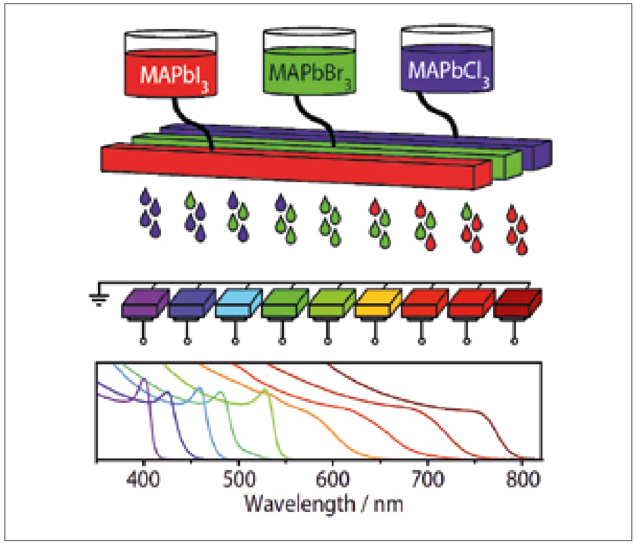
Using small-angle scattering at the PTB X-ray beamline of BESSY II, an HZB team led by Antonio Abate was able to experimentally investigate the colloidal chemistry of perovskite precursor solutions used for solar cell production. The results contribute to the targeted and systematic optimization of the manufacturing process and quality of these exciting inexpensive and versatile semiconductor materials.

arö

J. Mater. Chem. A. (2021): Small-angle scattering to reveal the colloidal nature of halide perovskite precursor solutions. Marion A. Flatken, Armin Hoell, Robert Wendt, Eneli Härk, André Dallmann, Albert Prause, Jorge Pascual, Eva Unger, and Antonio Abate. **DOI: 10.1039/D1TA01468D**

PEROVSKITE SPECTROMETER BY INKJET PRINTING

Metal halide perovskites are fascinating to researchers in academia and industry with the large range of possible applications in optoelectronics and photovoltaics. The fabrication of electronic components with this material is particularly appealing, because it is possible from solution, i.e. from an ink. Commercially available salts are dissolved in a solvent and then deposited on a substrate. Researchers from Innovation Lab HySPRINT at HZB and Humboldt Universität zu Berlin have used an advanced inkjet printing technique to produce a large range of photodetector devices based on a hybrid perovskite semiconductor. By mixing of only three inks, they were able to precisely tune the semiconductor properties during the printing process. Inkjet printing is an established fabrication method in industry, allowing fast and cheap solution processing. Extending the inkjet capabilities from large area coating towards combinatorial material synthesis opens the door for new possibilities for the fabrication of different electronic components in a single printing step.



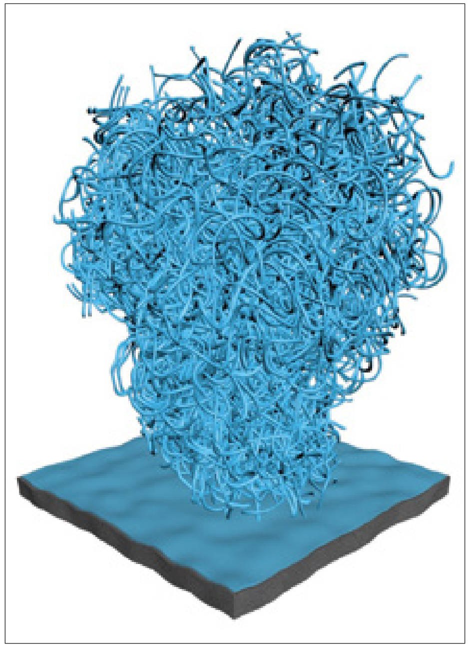
Three perovskite precursor inks can be used to print different metal halide perovskites. © DOI: 10.1002/adem.202101111

V. Schröder / F. Hermerschmidt

Advanced Engineering Materials (2021): Using Combinatorial Inkjet Printing for Synthesis and Deposition of Metal Halide Perovskites in Wavelength-Selective Photodetectors. Vincent R. F. Schröder, Felix Hermerschmidt, Sabrina Helper, Carolin Rehermann, Giovanni Ligorio, Hampus Näsström, Eva L. Unger, Emil J. W. List-Kratochvil. **DOI: 10.1002/adem.202101111**

ON THE TRAIL OF DESTRUCTIVE LITHIUM DENDRITES

Dendrites can form inside lithium batteries. These small needles or trees resemble the branched extensions of our nerve cells, from which they get their name. Dendrites form when the ions of an alkali metal like lithium encounter tiny crystallisation nuclei as the ions migrate back and forth between the internal plus and minus poles of a battery during the charge/discharge cycles. These dendrites grow during each charge/discharge cycle and eventually short-circuit the battery, destroying it – and in some cases even causing an explosion. It is not yet clear how this danger can be averted, and how the service life of energy storage devices can be increased, because we do not yet fully understand how the dendrites develop and grow.



During the operation of conventional battery storage, the tree-like lithium dendrites grow continuously and can cause irreparable damage in batteries. © I. Manke/HZB, K. Dong

To unravel the mystery of this nucleation and growth of dendrites in lithium-ion batteries, a research team took a look deep inside a battery using two specialised methods at the HZB. Using focussed ion-beam scanning electron microscopy and cryogenic transmission electron microscopy obtained high-resolution images of the internal lithium deposits accurate in every detail. These three-dimensional images represent a milestone in understanding the mechanisms at work during deposition.

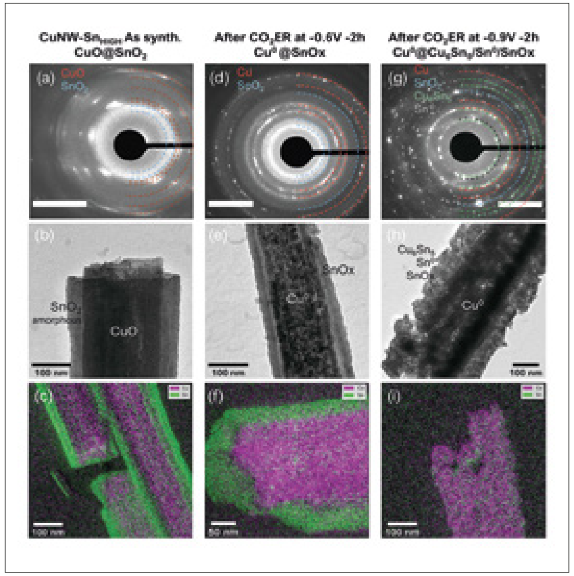
Kai Dürfeld

ACS Energy Letter (2021): Unravelling the Mechanism of Lithium Nucleation and Growth and the Interaction with the Solid Electrolyte Interface. K. Dong, Y. Xu, J. Tan, M. Osenberg, F. Sun, Z. Kochovski, D. Tung Pham, S. Mei, A. Hilger, E. Ryan, Y. Lu, J. Banhart, and I. Manke. **DOI: 10.1021/acsenergylett.1c00551**

PROCESSES IN COPPER-TIN CATALYSTS DECODED

The climate-damaging gas CO_2 can be converted electrochemically into useful raw materials for industry. However, this requires catalysts that are stable over a long period of time. Bimetallic copper-tin catalysts enable selective CO_2 reduction, producing either carbon monoxide or formate. An international research group at HZB has investigated copper-tin catalysts made from oxides that can be tuned to produce carbon monoxide or formate. The aim was to understand the complex interactions of copper and tin that lead to the different end products in catalysis. The research group found that the two metals change significantly during the electroreduction of CO_2. The dynamically changing mass and surface structures could be revealed by the variety of precise measurement methods available at HZB. The result: Both during the reduction of CO_2 to carbon monoxide and that to formate, the copper of the catalyst is transformed into metallic Cu_0. The content of tin dioxide in the catalyst is decisive for the question of which end product comes out at the end of the catalysis.

cn



Using three different measurement methods, the researchers tracked the dynamic changes of copper and tin in catalysts for the electroreduction of CO_2.

© DOI: 10.1002/aenm.202103328

Advanced Energy Materials (2021): Determining Structure-Activity Relationships in Oxide Derived Cu-Sn Catalysts During CO_2 Electroreduction Using X-Ray Spectroscopy. L. C. Pardo Pérez, A. Arndt, S. Stojkovikj, I. Y. Ahmet, J. T. Arens, F. Dattila, R. Wendt, A. Guilherme Buzanich, M. Radtke, V. Davies, K. Höflich, E. Köhnen, P. Tockhorn, R. Golnak, J. Xiao, G. Schuck, M. Wollgarten, N. López, and M. T. Mayer. **DOI: 10.1002/aenm.202103328**

SOLAR HYDROGEN FOR ANTARCTICA

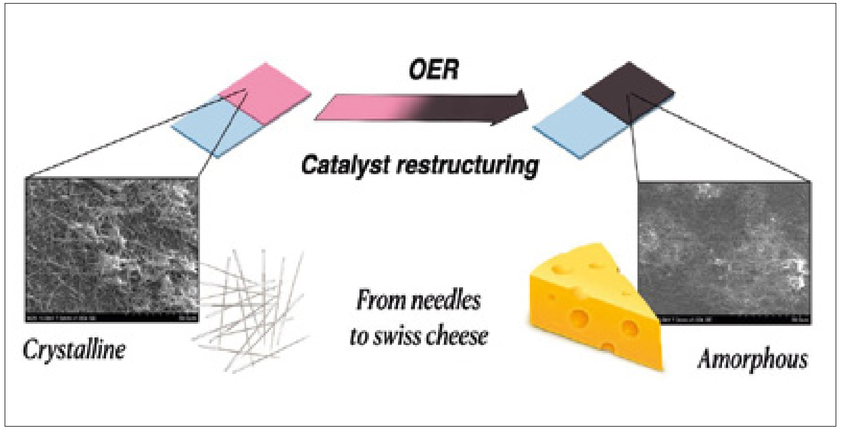
A team from the Helmholtz-Zentrum Berlin, Ulm University, and Heidelberg University has now investigated how hydrogen can be produced at the South Pole using sunlight, and which method is the most promising. The starting point was a research visit to Antarctica by environmental physicist Kira Rehfeld, University of Heidelberg. She was struck by the region's intense light, which could theoretically be used to produce hydrogen. "Our idea was to use solar modules to produce climate-neutral hydrogen on site during the Antarctic summer by splitting water into hydrogen and oxygen through electrolysis", says Matthias May, then a postdoc at the Institute for Solar Fuels of HZB. To do this, the research team empirically compared two different approaches: a conventional

Research stations like Neumayer III in Queen Maud Land, Antarctica, operated by the Alfred Wegener Institute of the Helmholtz Association, could use polar-generated hydrogen as an energy source in the future.

setup in which the photovoltaic module is thermally and physically separated from the electrolysis tank, and a newer, thermally coupled setup in which the photovoltaic module is in close contact with the wall of the electrolysis tank, promoting thermal diffusion. The results of this study, funded by the Volkswagen Foundation, confirm that thermally coupled systems have a potentially higher efficiency than thermally decoupled ones. Whether these advantages can be exploited economically, however, remains to be seen. *arö*

Energy & Environmental Science (2021): Efficiency gains for thermally coupled solar hydrogen production in extreme cold. Moritz Kölbach, Kira Rehfeld, and Matthias M. May. **DOI: 10.1039/D1EE00650A**

WHY DO CERTAIN CATALYSTS IMPROVE IN OPERATION?



Schematic of the electrochemical restructuring of erythrite. The fine needle-like structure melts during the conversion from a crystalline material to an amorphous one, which is porous like a Swiss cheese.

As a rule, most catalyst materials that generate oxygen during electrolytic water splitting in the production of hydrogen deteriorate during repeated catalytic cycles – they age. But there are also compounds that increase their performance over the course of catalysis. One example is the mineral erythrite, a mineral compound comprising cobalt and arsenic oxides. Now, a team led by Marcel Risch at BESSY II has discovered that two opposing developments are responsible for this. On the one hand, the catalytic activity of the individual catalysis centres decreases in the course of electrolysis, but at the same time the morphology of the catalyst layer also changes. Under favourable conditions, considerably more catalysis centres come into contact with the electrolyte as a result, so that the overall performance of the catalyst can increase. Marcel Risch has a vivid explanation for this: "Over time, the material becomes like Swiss cheese with many holes and a large surface area where many more reactions can take place." The loss of activity is overcompensated by the increasing number of reactions. Risch suggests that such mechanisms can also be found in many other classes of materials consisting of non-toxic compounds, which can be developed into suitable catalysts. *arö*

Advanced Energy Materials (2021): Requirements for beneficial electrochemical restructuring: A model study on a cobalt oxide in selected electrolytes. J. Villalobos, D. González-Flores, R. Urcuyo, M. L. Montero, G. Schuck, P. Beyer, M. Risch. **DOI: 10.1002/aenm.202101737**

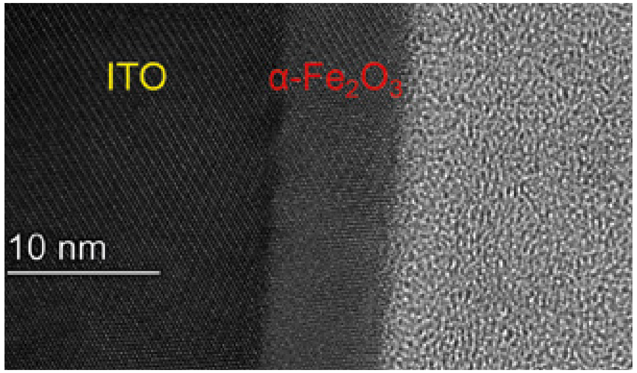
GREEN HYDROGEN: "RUST" AS A PHOTOANODE AND ITS LIMITS

Metal oxides such as rust are intriguing photoelectrode materials for the production of green hydrogen with sunlight. They are cheap and abundant, but in spite of decades of research, progress has been limited. A team at HZB, together with partners from Ben Gurion University and the Technion, Israel, has now analysed the optoelectronic properties of rust (haematite) and other metal oxides in unprecedented detail. The group at Technion investigated how the wavelength of absorbed light in hematite thin films affects the photoelectrochemical properties, while the HZB team determined the wavelength dependent charge carrier properties in thin films of rust with time-resolved microwave measurements.

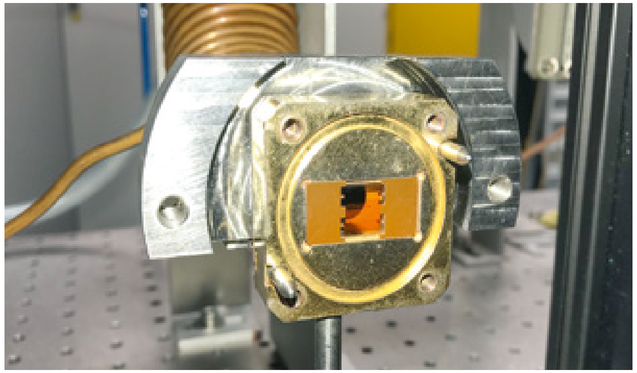
By combining their results, the researchers succeeded in extracting a fundamental physical property of the material that had generally been neglected when considering inorganic solar absorbers: The photogeneration yield spectrum. "Roughly speaking, this means that only part of the energy of the light absorbed by haematite generates mobile charge carriers, the rest generates rather localised excited states and is thus lost," Daniel Grave from Ben Gurion University explains.

Rust will not get much better

"This new approach provides experimental insight into light-matter interaction in haematite and allows distinguishing its optical absorption spectrum into productive absorption and non-productive absorption," Avner Rothschild from Technion explains. "We could show that the effective upper limit for the conversion efficiency of haematite photoanodes is significantly lower than that expected based on above band-gap absorption," says Grave. According to the new calculation, today's "champion" haematite photoanodes have already come quite close to the theoretically possible maximum. So it doesn't get much better than this.



Rust would be an extremely cheap and stable photoelectrode material to produce green hydrogen with light. But the efficiency is limited. The TEM image shows a photoanode containing a thin photoactive layer of rust. © Technion



The HZB team was able to determine the photoconductivity in the thin layers of rust using time-resolved microwave measurements; here is a picture of the measurement setup. © HZB

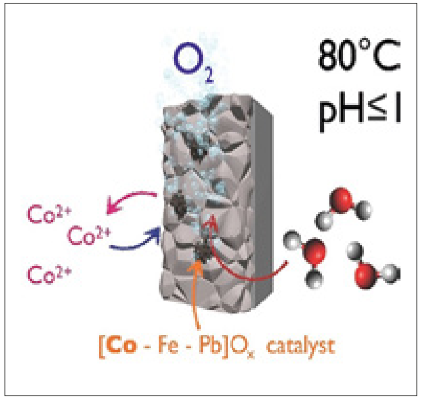
Assessing new photoelectrode materials

The approach has also been successfully applied to TiO_2, a model material, and $BiVO_4$, which is currently the best-performing metal oxide photoanode material.

"With this new approach, we have added a powerful tool to our arsenal that enables us to identify the realizable potential of photoelectrode materials. Implementing this to novel materials will hopefully expedite the discovery and development of the ideal photoelectrode for solar water splitting. It would also allow us to 'fail quickly', which is arguably just as important when developing new absorber materials," says Dennis Friedrich from HZB Institute for Solar Fuels. *arö*

Nature Materials (2021): Extraction of mobile charge carrier photogeneration yield spectrum of ultrathin-film metal oxide photoanodes for solar water splitting. Daniel A. Grave, David S. Ellis, Yifat Piekner, Moritz Kölbach, Hen Dotan, Asaf Kay, Patrick Schnell, Roel van de Krol, Fatwa F. Abdi, Dennis Friedrich and Avner Rothschild.
DOI: 10.1038/s41563-021-00955-y

CATALYST STABILITY VIA A COBALT-SELECTIVE SELF-HEALING MECHANISM



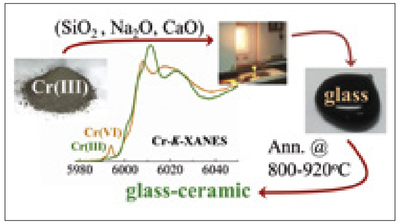
With the [Co-Fe-Pb]O_x anode catalyst for the oxidation of water, hydrogen could be produced at low cost.

© DOI: 10.1002/anie.202104123

The instability and expense of anodes for water electrolyzers with acidic electrolytes can be overcome through the implementation of a cobalt-iron-lead oxide electrocatalyst. The reason for this is a self-healing process of the catalyst in the presence of dissolved metal precursors. The permanent operation of such a catalyst has been demonstrated by an international team of researchers at BESSY II. *cn*

Angewandte Chemie (2021): Stable Acidic Water Oxidation with a Cobalt–Iron–Lead Oxide Catalyst Operating via a Cobalt-Selective Self-Healing Mechanism. D. Simondson, M. Chatti, S. A. Bonke, M. F. Tesch, R. Golnak, J. Xiao, D. A. Hoogeveen, P. V. Cherepanov, J. L. Gardiner, A. Tricoli, D. R. MacFarlane, A. N. Simonov. **DOI: 10.1002/anie.202104123**

CHROMIUM IN STABILIZED TANNERY WASTES



X-ray absorption fine structure spectroscopy (XAFS) was used to investigate the effective stabilisation of tannery sludge wastes.

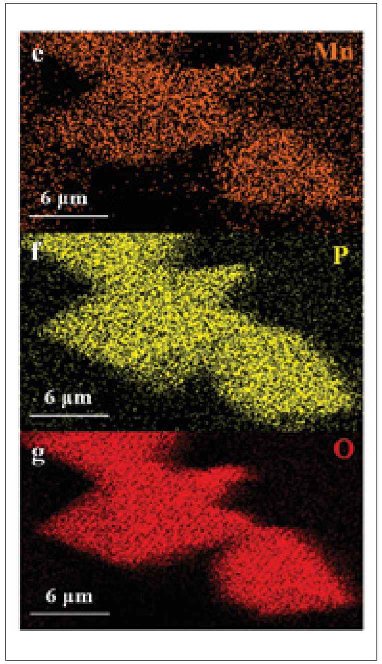
© DOI: 10.1016/j.jhazmat.2020.123734

In contrast to the less harmful chromium III compounds, so-called chromium VI compounds, such as those produced during the tanning of leather, are allergenic to acutely toxic, depending on the dosage. A Greek research group at the Aristotle University of Thessaloniki has shown at HZB with the help of X-ray absorption fine structure spectroscopy (XAFS) that the effective reduction of Cr(VI) and the structural role of Cr strongly depend on the chemical composition of the waste. *cn*

Journal of Hazardous Materials (2021): Probing the structural role of Cr in stabilized tannery wastes with X-ray absorption fine structure spectroscopy. F. Pinakidou, M. Katsikini, S. Varitis, Ph. Komninou, G. Schuck, E.C. Paloura. **DOI: 10.1016/j.jhazmat.2020.123734**

A STABLE MANGANESE-BASED CATALYST FOR HYDROGEN PRODUCTION

One of the key catalytic reactions for life on earth, the oxidation of water to molecular oxygen, occurs in the oxygen-evolving complex of the photosystem II (PSII) mediated by a manganese-containing cluster. In order to artificially reproduce this process and use it for the production of hydrogen as a regenerative energy carrier in large quantities, considerable research efforts are being carried out worldwide on manganese-based catalysts. So far, their unsatisfying catalytic performance and poor stability have been a fundamental. An international research team has for the first time developed a manganese-based anode material that combines electrocatalytic water oxidation and the selective oxygenation of organic substances with the highest efficiency to date. They achieved this by using spiral-shaped manganese borophosphates, which represent a new class of materials. The uniquely high catalytic activity and durability (more than five months) of the material in alkaline media are due to their unexpected surface transformation into an amorphous MnO_x phase with a birnessite-like short-range order and surface-stabilised MnIII sites under extended electrical bias. The team was able to demonstrate this process using a combination of in situ Raman and quasi in situ X-ray absorption spectroscopy as well as ex situ methods at the X-ray source BESSY II at HZB. *cn*



EDX mapping of hexagonal LiMnBPO crystals in which a uniform distribution of manganese (orange), phosphorus (yellow) and oxygen (red) was achieved, confirming the phase purity of the product.

© DOI: 10.1002/adma.202004098

Advanced Materials (2021): Combination of Highly Efficient Electrocatalytic Water Oxidation with Selective Oxygenation of Organic Substrates using Manganese Borophosphates. Prashanth W. Menezes, Carsten Walter, Biswarup Chakraborty, Jan Niklas Hausmann, Ivelina Zaharieva, Achidi Frick, Elizabeth von Hauff, Holger Dau, Matthias Driess. **DOI: 10.1002/adma.202004098**

HIGHLIGHTS FROM OUR RESEARCH – INFORMATION

Intensive basic research is being conducted at HZB in the field of information technologies. The aim is to gain a better understanding of processes and structures at the atomic level or of electron spins. This knowledge can be used to improve the storage capacities and energy consumption of information technology and to open up new areas of application. **There is a more detailed text on almost every news item in the HZB Newsroom. Click on this symbol: ➲ In our newsroom you will also find other news from our research in the field of information.**

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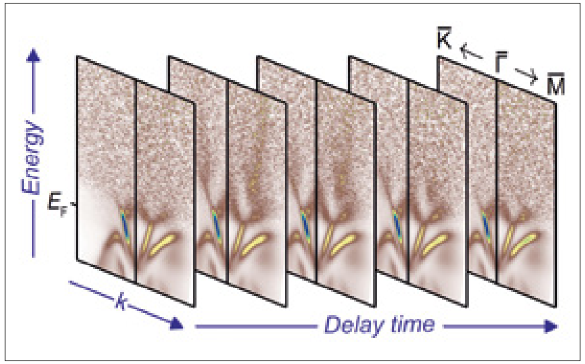
TOPOLOGICAL MATERIALS FOR ULTRAFAST SPINTRONICS



Snapshots of the electronic structure of Sb acquired with femtosecond time-resolution. Note the changing spectral weight above the Fermi energy (EF).
© DOI: 10.1038/s42005-021-00657-6

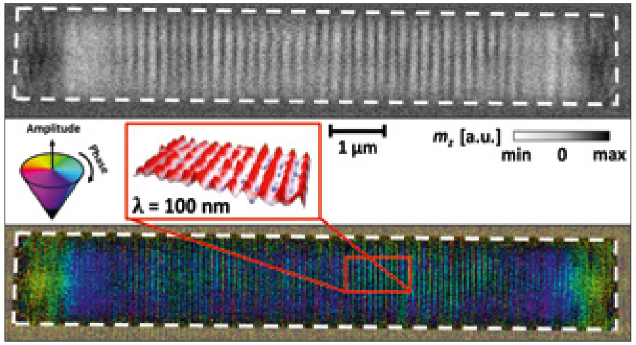
The laws of quantum physics rule the microcosm. They determine, for example, how easily electrons move through a crystal and thus whether the material is a metal, a semiconductor or an insulator. Quantum physics may lead to exotic properties in certain materials: In so-called topological insulators, only the electrons that can occupy some specific quantum states are free to move like massless particles on the surface, while this mobility is completely absent for electrons in the bulk. What's more, the conduction electrons in the „skin" of the material are necessarily spin polarized, and form robust, metallic surface states that could be utilized as channels in which to drive pure spin currents on femtosecond time scales (1 fs= 10^{-15} s).

A team led by HZB physicist Jaime Sánchez-Barriga has gained new insights into the ultrafast excitation of topological states of matter in single crystal antimony (Sb). Using time- and spin-resolved capabilities, the physicists at BESSY II investigated how the complex interplay in the dynamical behaviours of electrons from the bulk and the surface leads to unusual spin dynamics, following the ultrafast optical excitation. The work is an important step on the way to spintronic devices based on topological materials for ultrafast information processing.

arö

Nature Communication Physics (2021): Observation of a giant mass enhancement in the ultrafast electron dynamics of a topological semimetal. O. J. Clark, F. Freyse, I. Aguilera, A. S. Frolov, A. M. Ionov, S. I. Bozhko, L. V. Yashina, and J. Sánchez-Barriga. **DOI: 10.1038/s42005-021-00657-6**

THE WORLD'S FIRST VIDEO RECORDING OF A SPACE-TIME CRYSTAL



The greyscale image above shows a snapshot of the time-resolved X-ray microscopy of the magnonic space-time crystal. Its interactions with other magnons give rise to ultrashort spin waves, which are shown in the image below. Here, the colour space describes the phase, and the brightness the amplitude of the spin waves generated.
© MPI-IS

A crystal is a solid whose atoms or molecules are regularly arranged in a certain structure. It is similar with space-time crystals: however, the recurring structure does not only exist in space, but also in time. The smallest components are constantly in motion until they correspond exactly to the original arrangement pattern again after a certain period. In 2012, the Nobel Prize winner in physics Frank Wilczek discovered the symmetry of matter in time and made the assumption that research would soon be able to create space-time crystals.

A German-Polish research team has succeeded in creating a micrometre-sized space-time crystal of magnons at room temperature. With the help of the MAXYMUS scanning X-ray microscope at BESSY II, they were even able to film the periodic magnetisation structure in a crystal. The scientists from the Max Planck Institute for Intelligent Systems (MPI-IS) in Stuttgart, Adam Mickiewicz University and the Polish Academy of Sciences in Poznań presented this world's first video of a space-time crystal at room temperature and the research project itself in *Physical Review Letters*.

MPI-IS/red.

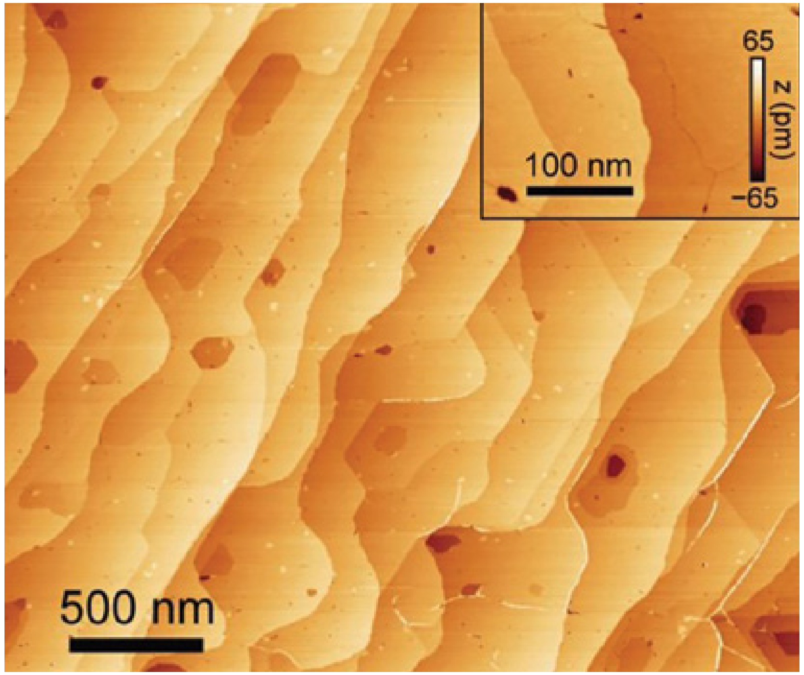
Phys. Rev. Lett. (2021): Real-Space Observation of Magnon Interaction with Driven Space-Time Crystals. N. Träger, P. Gruszecki, F. Lisiecki, F. Groß, J. Förster, M. Weigand, H. Głowiński, P. Kuświk, J. Dubowik, G. Schütz, M. Krawczyk, and J. Gräfe. **DOI: 10.1103/PhysRevLett.126.057201**

SPINTRONICS: EXOTIC FERROMAGNETIC ORDER IN TWO-DIMENSIONS

The thinnest materials in the world are only a single atom thick. These kinds of two-dimensional or 2D materials are causing a great deal of excitement among research teams worldwide. This is because these materials promise unusual properties that cannot be obtained using three-dimensional materials. Structures known as van-der-Waals monolayers are arousing particular interest. These are combinations of two or more layers of different materials that are each only a single atom thick, with the layers held to one another by weak electrostatic van-der-Waals forces. By selecting the type and sequence of material layers bound in this way, specific electrical, magnetic, and optical characteristics can be chosen and modified. However, scaled-up homogeneous deposition of individual van-der-Waals layers having ferromagnetic properties has not yet been achieved.

Scientists from the Max Planck Institute for Microstructure Physics in Halle, Germany, the ALBA synchrotron light source in Barcelona, Spain, and HZB have now succeeded for the first time in creating a uniform two-dimensional material – and demonstrating an exotic ferromagnetic behaviour within it known as "easy-plane" magnetism. The researchers utilised chromium chloride ($CrCl_3$) as a material. The team's goal was to answer the question of how the magnetic order in chromium chloride manifests itself when it consists of only a single monoatomic layer.

The group achieved this by taking a detailed look at the magnetic properties of the 2D material. To do so, they used the unique capabilities of the VEKMAG vector magnet facility installed at HZB's synchrotron radiation source BESSY II. "Here it is possible to investigate samples using soft X-rays in a strong magnetic field – and at temperatures near absolute zero", says Florin Radu, head of the team at HZB responsible for operations at the VEKMAG facility. During the measurements, the researchers observed how ferromagnetic order formed in the two-dimensional material below a certain temperature, what is known as the Curie temperature. "In the monoatomic chromium chloride layer, a phase transition characteristic of easy-plane magnets took place that had never been observed before in such a 2D material," reports Bedoya-Pinto.



STM topography of a monolayer $CrCl_3$ grown on Graphene/6H-SiC(0001). Inset, a magnified topography image, which reveals the grain boundaries.

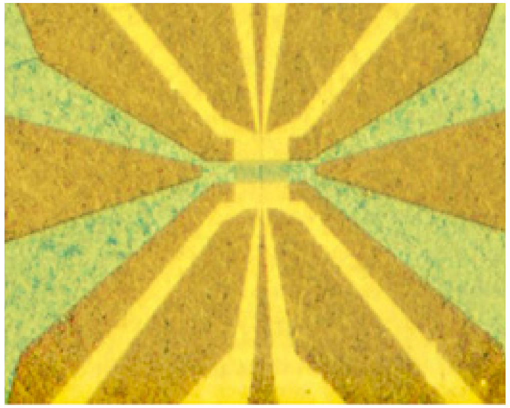
© DOI: 10.1126/science.abd5146

Tailwind for the development of spintronics

The discovery not only offers new insights into the magnetic behaviour of two-dimensional materials. "We now also have an excellent platform for exploring a variety of physical phenomena that only exist in two-dimensional magnets," Bedoya-Pinto is pleased to say, such as superfluid (lossless) transport of spin. These are the basis for a new form of data processing that is known as spintronics. In the future, it could enable significantly faster and energy-saving storage of data. *rb*

Science (2021): Intrinsic 2D-XY ferromagnetism in a van der Waals monolayer. Amilcar Bedoya-Pinto, Jing-Rong Ji, Avanindra Pandeya, Pierluigi Gargiani, Manuel Valvidares, Paolo Sessi, James Taylor, Florin Radu, Kai Chang and Stuart S.P. Parkin. **DOI: 10.1126/science.abd5146**

SUPERCONDUCTIVITY MEETS SPINTRONICS



Device where the long range Josephson coupling has been demonstrated. Superconducting $YBa_2Cu_3O_7$ regions (yellow) are separated by a half-metal $La_{2/3}Sr_{1/3}MnO_3$ ferromagnet (green).

© DOI: 10.1038/s41563-021-01162-5

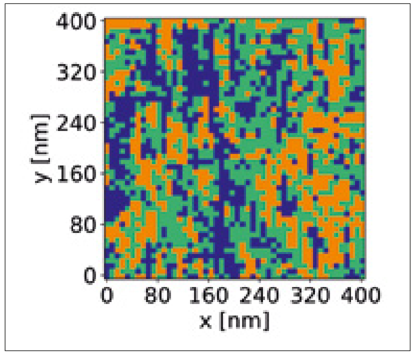
Superconducting coupling between two regions separated by a one micron wide ferromagnetic compound has been proved by an international team. This macroscopic quantum effect, known as Josephson effect, generates an electrical current within the ferromagnetic compound made of superconducting Cooper-pairs. With the help of magneto-transport measurements, the researchers were able to demonstrate the presence of a supercurrent circulating through the manganite – this supercurrent is arising from the superconducting coupling between both superconducting regions, and thus a manifestation of a Josephson effect with a macroscopic long range. In addition, they explored another interesting property: In superconductors electrons pair together in so-called Cooper pairs. In the vast majority of superconducting materials these pairs are composed by electrons with opposite spin in order to minimise the magnetic exchange field which is detrimental for the stabilisation of superconductivity. In the ferromagnetic material used here, measurements at BESSY II showed that the spin of the Cooper electrons is the same. The results point the way to superconducting spintronic applications with very low energy requirements, where spin-polarised currents are protected by quantum coherence. *red.*

Nature Materials (2021): Extremely long range, high-temperature Josephson coupling across a half metallic ferromagnet. D. Sanchez-Manzano, S. Mesoraca, F. Cuellar, M. Cabero, V. Rouco, G. Orfila, X. Palermo, A. Balan, L. Marcano, A. Sander, M. Rocci, J. García-Barriocanal, F. Gallego, J. Tornos, A. Rivera, F. Mompean, M. García-Hernández, J. M. González-Calbet, C. León, S. Valencia, C. Feuillet-Palma, N. Bergeal, A.I. Buzdin, J. Lesueur, Javier E. Villegas, and J. Santamaría. **DOI: 10.1038/s41563-021-01162-5**

A SHARP LOOK INTO TINY FERROELECTRIC CRYSTALS

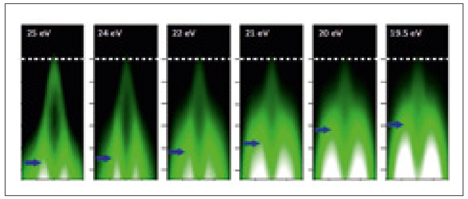
Ferroelectric materials have a special internal structure that could be used to store large amounts of data in a small space. But on the nanometre scale, ferroelectric polarisation changes. Now, a team led by Catherine Dubourdieu has demonstrated a way to map the polarisation pattern in thin ferroelectric layers precisely and also non-destructively. *rb*

ACS Appl. Electron. Mater. (2021): Sub-10 nm Probing of Ferroelectricity in Heterogeneous Materials by Machine Learning Enabled Contact Kelvin Probe Force Microscopy. S. W. Schmitt, R. K. Vasudevan, M. Seifert, A. Y. Borisevich, V. Deshpande, S. V. Kalinin, and C. Dubourdieu. **DOI: 10.1021/acsaelm.1c00569**



Map obtained for a thin barium titanate film after clustering the data measured by contact Kelvin probe force microscopy (cKPFM) by a machine learning method. From this map, scientists can obtain detailed information on ferroelectric domains. © HZB

DISORDER BRINGS OUT QUANTUM PHYSICAL TALENTS



The Dirac cone is typical for topological insulators and is practically unchanged on all six images (ARPES measurements at BESSY II). The blue arrow additionally shows the valence electrons in the volume. © HZB

Quantum effects are most noticeable at extremely low temperatures, which limits their usefulness for technical applications. Thin films of $MnSb_2Te_4$, however, show new talents due to a small excess of manganese. Apparently, the resulting disorder provides spectacular properties, as a group of researchers was able to prove by measurements at BESSY II. *arö*

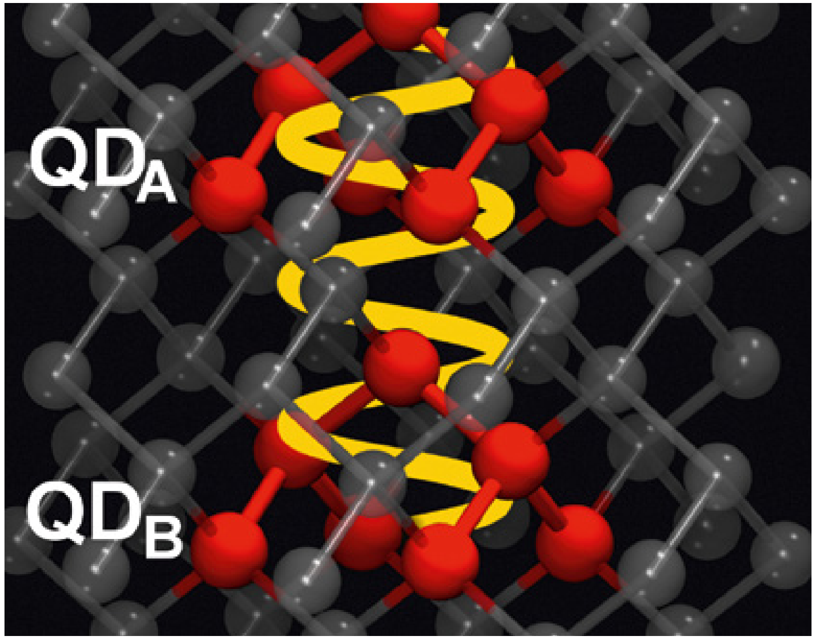
Advanced Materials (2021): Mn-rich $MnSb_2Te_4$: A topological insulator with magnetic gap closing at high Curie temperatures of 45-50 K. S. Wimmer, J. Sánchez-Barriga, P. Küppers, A. Ney, E. Schierle, F. Freyse, O. Caha, J. Michalička, M. Liebmann, D. Primetzhofer, B. Lake, E. V. Chulkov et. al. **DOI: 10.1002/adma.202102935**

HOW QUANTUM DOTS CAN “TALK” TO EACH OTHER

So-called quantum dots are a new class of materials with many applications. Quantum dots are realized by tiny semiconductor crystals with dimensions in the nanometre range. The optical and electrical properties can be controlled through the size of these crystals. As QLEDs, they are already on the market in the latest generations of TV flat screens, where they ensure particularly brilliant and high-resolution colour reproduction. However, quantum dots are not only used as “dyes”, they are also used in solar cells or as semiconductor devices, right up to computational building blocks, the qubits, of a quantum computer.

A team led by Annika Bande, head of the “Theory of Electron Dynamics and Spectroscopy” group at HZB, has extended the understanding of the interaction between several quantum dots with an atomistic view in a theoretical publication. Although quantum dots are extremely tiny nanocrystals, they consist of thousands of atoms with, in turn, multiples of electrons. Even with supercomputers, the electronic structure of such a semiconductor crystal could hardly be calculated, emphasises the theoretical chemist, who recently completed her habilitation at Freie Universität. “But we are developing methods that describe the problem approximately,” Bande explains. “In this case, we worked with scaled-down quantum dot versions of only about a hundred atoms, which nonetheless feature the characteristic properties of real nanocrystals.”

With this approach, after a year and a half of development and in collaboration with Jean Christophe Tremblay from the CNRS-Université de Lorraine in Metz, the group succeeded in simulating the interaction of two quantum dots, each made of hundreds of atoms, which exchange energy with each other. Specifically, they have investigated how these two quantum dots can absorb, exchange and permanently store the energy controlled by light. A first light pulse is used for excitation, while the second light pulse induces the storage.



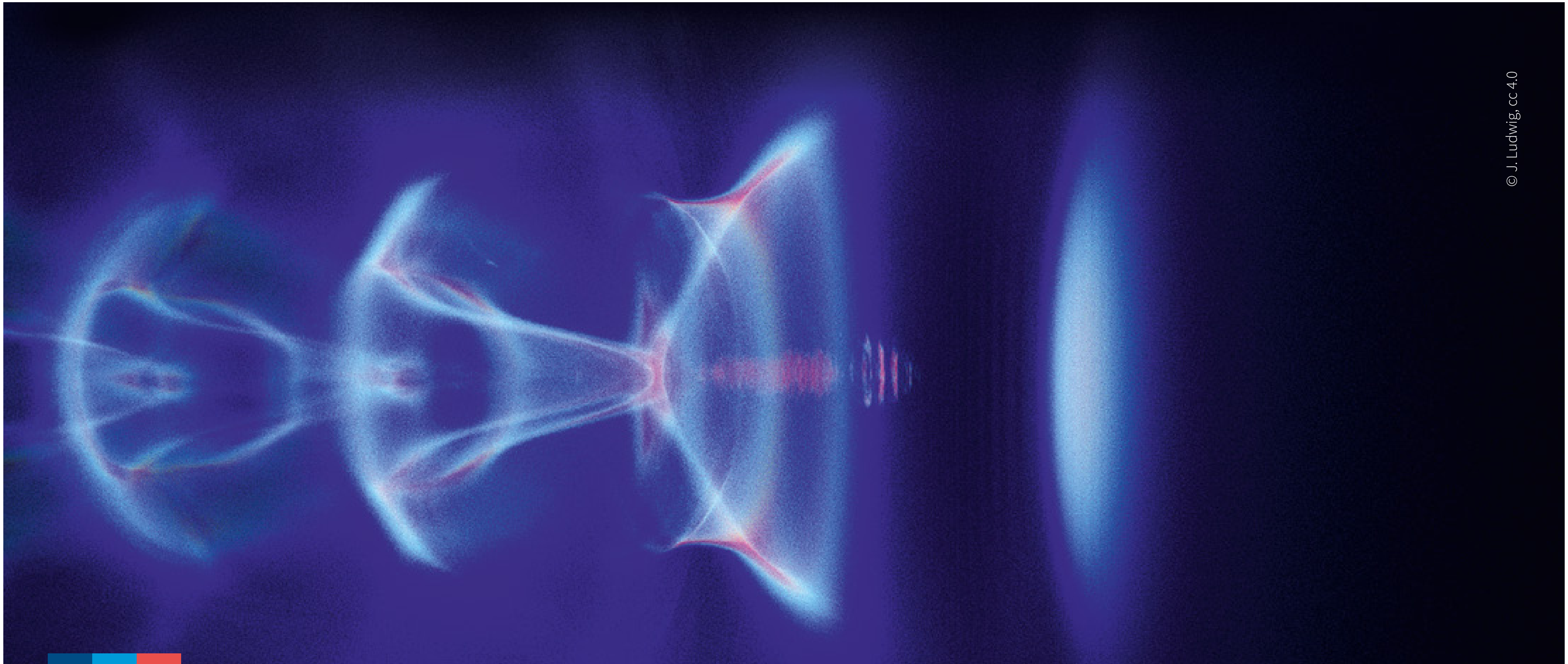
The illustration shows two quantum dots “communicating” with each other by exchanging light. © HZB

Electron structure calculated with the highest precision

In total, three different pairs of quantum dots were investigated to capture the effect of size and geometry. The researchers calculated the electron structure with the highest precision and simulated the electronic motion in real time at femtosecond resolution (10^{-15} s). The results are also very useful for experimental research and development in many fields of application, for example for the development of qubits or to support photocatalysis, to produce green hydrogen gas by sunlight. “We are constantly working on extending our models towards even more realistic descriptions of quantum dots,” says Bande, “for example to capture the influence of temperature and environment.”

Pascal Krause

J. Phys. Chem. A (2021): Atomistic Simulations of Laser-controlled Exciton Transfer and Stabilization in Symmetric Double Quantum Dots. Pascal Krause, Jean Christophe Tremblay, and Annika Bande. **DOI: 10.1021/acs.jpca.1c02501**



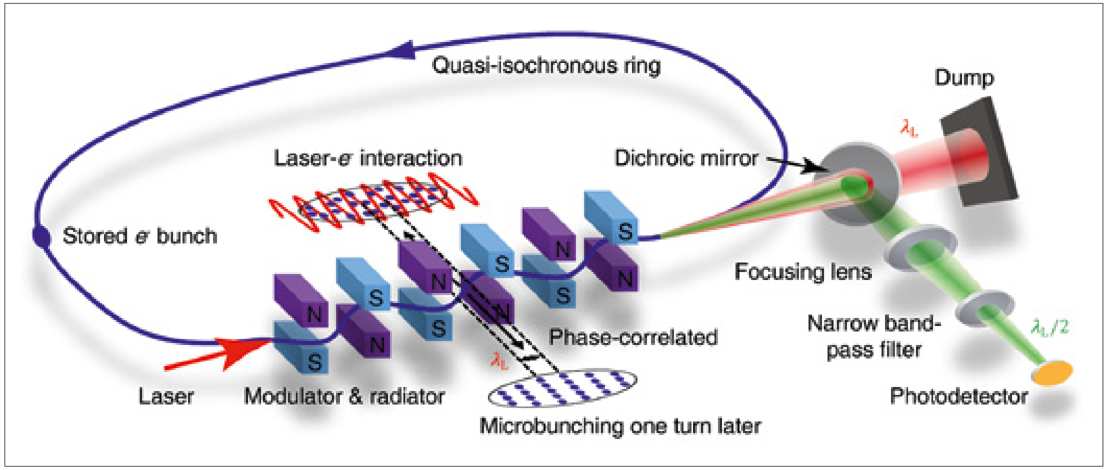
HIGHLIGHTS FROM OUR RESEARCH – MATTER

To enable deep insights into matter, the X-ray source BESSY II and its instruments are constantly being further developed. Groups from accelerator physics and materials research are working on this. The versatile measuring instruments and powerful operation of BESSY II enable first-class materials research at HZB and attract numerous research guests to Berlin from Germany and abroad. **There is a more detailed text on almost every news item in the HZB Newsroom. Click on this symbol: ➲ In our newsroom you will also find other news from our research in the field of matter.**

NEW OPTIONS FOR SYNCHROTRON LIGHT SOURCES

The most modern light sources for research are based on particle accelerators. These are large facilities in which electrons are accelerated to almost the speed of light, and then emit light pulses of a special character. In storage-ring-based synchrotron radiation sources such as BESSY II, the electron bunches travel in the ring for billions of revolutions, then generate a rapid succession of very bright light pulses in the deflecting magnets. In contrast, the electron bunches in free-electron lasers (FELs) are accelerated linearly and then emit a single super-bright flash of laser-like light. Storage ring sources as well as FEL sources have facilitated advances in many disciplines in recent years, from deep insights into biological and medical questions to materials research, technology development, and quantum physics.

Accelerator experts from HZB, the German federal metrology institute Physikalisch-Technische Bundesanstalt (PTB), and Tsinghua University in Beijing have shown that a pattern of pulses can be generated in a synchrotron radiation source that combines the advantages of both systems. The synchrotron source delivers short, intense microbunches of electrons that produce radiation pulses having a laser-like character (as with FELs), but which can also follow each other closely in sequence (as with synchrotron light sources).



Experimental setup. The stored electron bunches are modulated by a laser in an undulator. They become micro-bunched after one complete revolution in the storage ring and produce coherent radiation.

Creation of microbunches

The idea was developed about ten years ago under the catchphrase „Steady-State Microbunching“ (SSMB) by leading accelerator theorist Alexander Chao and his PhD student Daniel Ratner at Stanford University. The German-Chinese research group has succeeded in experimentally confirming the SSMB principle. The HZB and PTB experts used an optical laser whose light wave was coupled in precise spatial and temporal synchronisation with the electron bunches in the MLS. This modulated the energies of the electrons in the bunches. “That causes the electron bunches, which are a few millimetres long, to split into microbunches of only one micrometre length after exactly one revolution in the storage ring, and then to emit light pulses that coherently amplify each other like in a laser”, explains Jörg Feikes, accelerator physicist at HZB. “The empirical detection of the coherent radiation was anything but easy, but our PTB colleagues developed an innovative optical detection unit with which it was successful.”

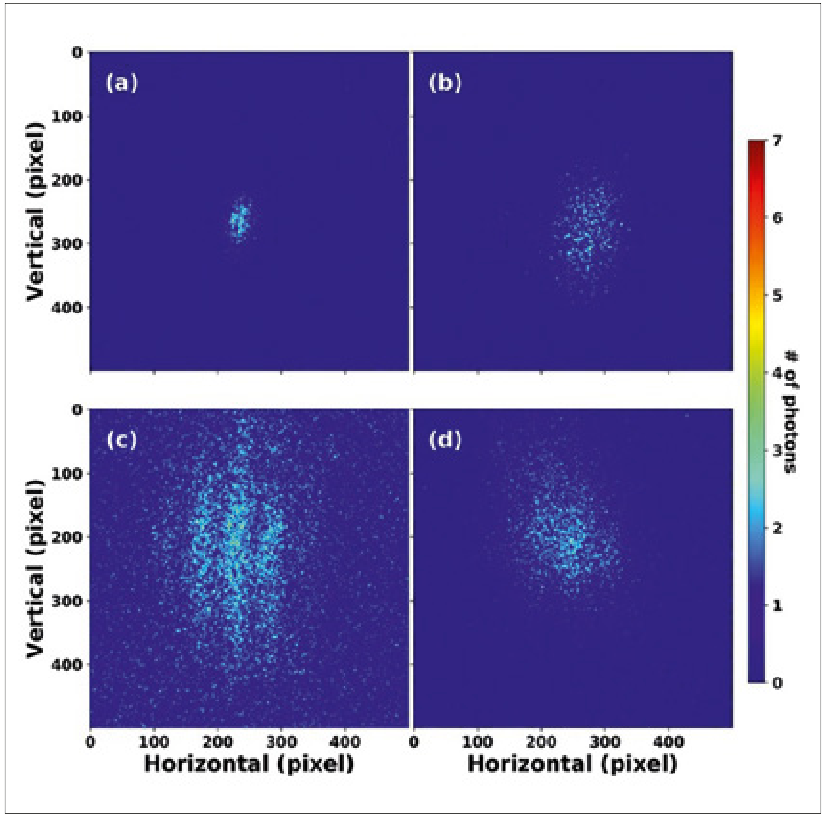
Combining the virtues of both systems

“In the final stage, an SSMB source could provide radiation of a new character. The pulses are intense, focused, and narrow-band. They combine the advantages of synchrotron light with the advantages of FEL pulses, so to speak,” explains Markus Ries, accelerator expert at HZB. This radiation is potentially suitable for industrial applications. *arö*

Nature (2021): Experimental demonstration of the mechanism of steady-state microbunching. Xiujie Deng, Alexander Chao, Jörg Feikes, Arne Hoehl, Wenhui Huang, Roman Klein, Arnold Kruschinski, Ji Li, Aleksandr Matveenko, Yuriy Petenev, Markus Ries, Chuanxiang Tang and Lixin Yan. **DOI: 10.1038/s41586-021-03203-0**

BEAM DIAGNOSTICS FOR FUTURE LASER WAKEFIELD ACCELERATORS

For decades, particle accelerators have been getting bigger and bigger. In the meantime, ring accelerators with circumferences of many kilometres have reached a practical limit. Linear accelerators in the gigahertz range also require very long construction lengths. For some years now, however, an alternative is explored: „tabletop particle accelerators“ based on the laser excitation of charge waves in plasmas (laser wakefield): A high-power laser excites a charge wave in a plasma, which propagates at the speed of the laser pulse and pulls electrons behind it in its „wake“, thus accelerating them. Electron energies in the giga-electron-volt range have been achievable with this technique for some time. However, the electron bunches produced in this way have so far been too small and too poorly focused to use the synchrotron radiation they emit for research.



Information on beam quality can be extracted via the interference patterns at different focal lengths and photon intensities. © DOI: 10.1038/s42005-021-00717-x

Precise measurement of electron bunches

For the further development of the technology, a method is therefore needed to precisely measure and control the cross-section and quality of the electron bunches individually. The storage ring of the German federal metrology institute Physikalisch-Technische Bundesanstalt (PTB), the Metrology Light Source (MLS), allows the generation of small electron bunches in flexible research operation. They are very similar to those of laser wakefield accelerators. However, their properties can be easily reproduced and precisely adjusted and varied. A team at HZB and PTB has now developed a method to measure the lateral expansion of the electron beam of a laser plasma accelerator with a resolution in the micrometre range.

Test under realistic conditions

“To do this, we use a technique that is successfully employed at the BESSY II storage ring,” explains Thorsten Kamps, co-author of the study. First author Ji-Gwang Hwang had the idea of using the coherent radiation of electron pulses in the visible range via the phenomenon of interference (double slit) and determining the beam cross-section as a deviation from a perfect point source. With the help of a highly sensitive camera and complex algorithms, the team succeeded in measuring the lateral beam size in the range of a few micrometres. Katharina Albrecht carried out the measurements as part of her bachelor‘s thesis in physics. “We worked very closely with our colleagues from the MLS at PTB for this project,” Kamps emphasises. “There, it is possible to imitate the electron beam from a plasma accelerator on a beamline and thus test the method under realistic conditions,” says Kamps. *arö*

Communications Physics (2021): Monitoring the size of low-intensity beams at plasma-wakefield accelerators using high-resolution interferometry. Ji-Gwang Hwang, Katharina Albrecht, Arne Hoehl, Beñat Alberdi Esuain, and Thorsten Kamps. **DOI: 10.1038/s42005-021-00717-x**

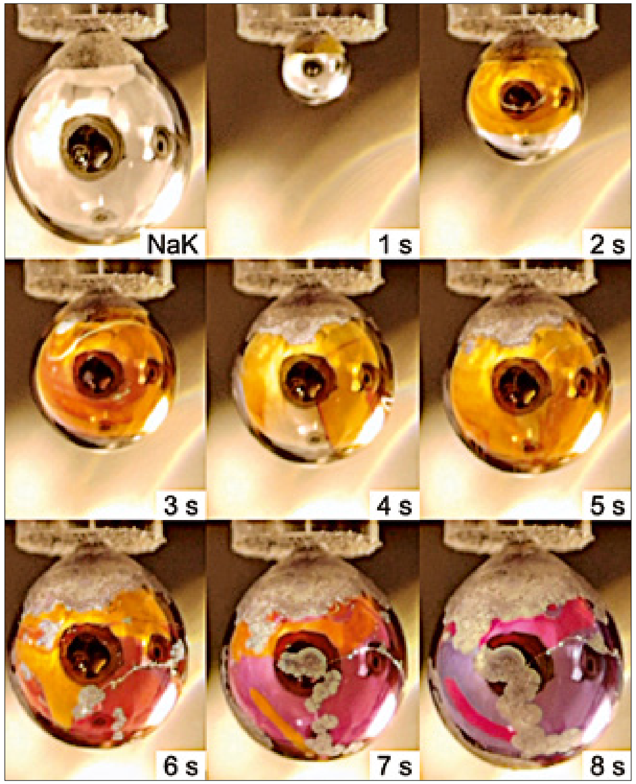
WATER AS A METAL – DETECTED AT BESSY II

Pure, distilled water is an almost perfect insulator. It consists of H_2O molecules that are loosely linked to one another via hydrogen bonds. The valence electrons remain bound and are not mobile. To create a conduction band with freely moving electrons, water would have to be pressurised to such an extent that the orbitals of the outer electrons overlap. However, a calculation shows that this pressure is only present in the core of large planets such as Jupiter.

An international collaboration of 15 scientists from eleven research institutions has now used a completely different approach to produce an aqueous solution with metallic properties for the first time and documented this phase transition at BESSY II. To do this, they experimented with alkali metals, which release their outer electron very easily. They put a tiny bit of water on a drop of alkali metal, a sodium-potassium (Na-K) alloy, which is liquid at room temperature. At BESSY II, they set up the experiment in the SOL^3PES high vacuum sample chamber at the U49/2 beamline.

An extremely thin skin of water vapour

The sample chamber contains a fine nozzle from which the liquid Na-K alloy drips. The silver droplet grows for about ten seconds until it detaches from the nozzle. As the droplet grows, some water vapour flows into the sample chamber and forms an extremely thin skin on the surface of the droplet, only a few layers of water molecules. This almost immediately causes the electrons as well as the metal cations to dissolve from the alkali alloy into the water. The released electrons in the water behave like free electrons in a conduction band.



After about five seconds, a thin film of metallic water has formed around the sodium-potassium drop, recognisable by the golden shimmer. © HZB

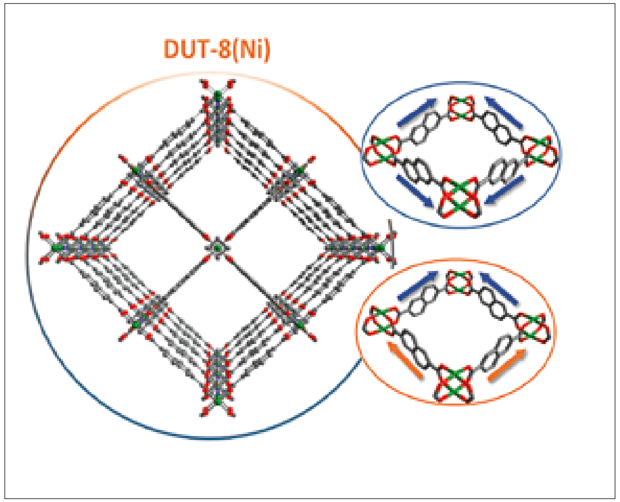
From silver to gold

"You can see the phase transition to metallic water with the naked eye. The silvery sodium-potassium droplet covers itself with a golden glow, which is very impressive," reports Robert Seidel, who supervised the experiments at BESSY II. The thin layer of gold-coloured metallic water remains visible for a few seconds. This enabled the team led by Pavel Jungwirth, Czech Academy of Sciences, Prague, to prove with spectroscopic analyses at BESSY II and at the IOCB in Prague that it is indeed water in a metallic state.

The two decisive fingerprints of a metallic phase are the plasmon frequency and the conduction band. The groups were able to determine these two quantities using optical reflection spectroscopy and X-ray photoelectron spectroscopy: While the plasmon frequency of the gold-coloured, metallic "water skin" is about 2.7 eV (i.e. in the blue range of visible light), the conduction band has a width of about 1.1 eV with a sharp Fermi edge. "Our study not only shows that metallic water can indeed be produced on Earth, but also characterises the spectroscopic properties associated with its beautiful golden metallic luster," says Seidel. *arö*

Nature (2021): Spectroscopic Evidence for a Gold-Coloured Metallic Water Solution. P. E. Mason, H. C. Schewe, T. Buttersack, V. Kostal, M. Vitek, R. S. McMullen, H. Ali, F. Trinter, C. Lee, D. M. Neumark, S. Thürmer, R. Seidel, B. Winter, S. E. Bradforth, and P. Jungwirth.
DOI: 10.1038/s41586-021-03646-5

NEW INSIGHTS INTO SWITCHABLE MOF STRUCTURES AT THE MX BEAMLINES

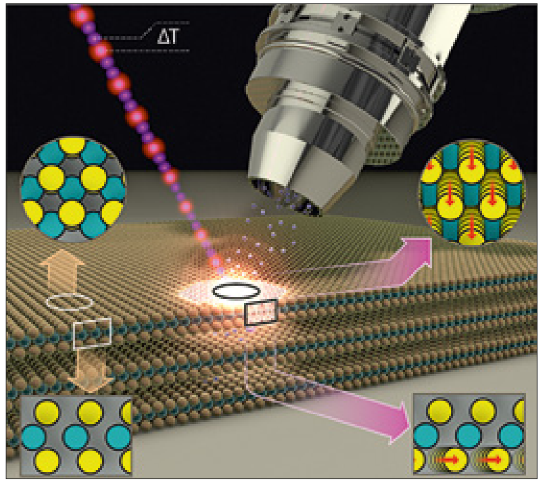


View into a MOF crystal exemplified by DUT-8. The massive pores are clearly discernible. © TU Dresden

Metal-organic framework compounds (MOFs) consist of inorganic and organic groups and are characterised by a large number of pores into which other molecules can be incorporated. MOFs are therefore interesting for many applications, for example for the storage of gases, but also for substance separation, sensor technology or catalysis. Some of these MOF structures react to different guest molecules by changing their structures. They are thus considered switchable. One of these is “DUT-8”, a material that has now been investigated by a team led by Stefan Kaskel from the Technical University Dresden at the MX beamlines of BESSY II. “MOF crystals have many things in common with protein crystals,” says HZB expert Manfred Weiss, who heads the MX team. “The diffraction patterns that DUT-8 showed on the MX beamlines at HZB were extremely complex. We were now able to attribute this to various transitions between ordered and less ordered phases,” explains Kaskel. The enclosed guest molecule directs the network into one of over a thousand possible disorder configurations. The results contribute to a better understanding of switching processes and gas exchange reactions in such MOF structures. *red.*

Nature Chemistry (2021): Adaptive response of a metal–organic framework through reversible disorder–disorder transitions. S. Ehrling, E. M. Reynolds, V. Bon, I. Senkovska, T. E. Gorelik, J. D. Evans, M. Rauche, M. Mendt, Manfred S. Weiss, A. Pöppl, E. Brunner, U. Kaiser, A. L. Goodwin and S. Kaskel. **DOI: 10.1038/s41557-021-00684-4**

HOW LIGHT ACTIVATES MoS_2 LAYERS TO BECOME CATALYSTS



A light pulse triggers in molybdenum-sulfide thin films a phase transition from the semiconducting to the metallic phase and thus enhances the catalytic activity. © M. Künsting/HZB

MoS_2 thin films of superposed alternating layers of molybdenum and sulfur atoms form a two-dimensional semiconducting surface. However, even a surprisingly low-intensity blue light pulse is enough to alter the properties of the surface and make it metallic. The exciting thing is that the MoS_2 layers in this metallic phase are also particularly active catalytically. They can then be employed, for example, as inexpensive catalysts for the production of hydrogen. Physicist Nomi Sorgenfrei and her team have constructed a new instrument at BESSY II to precisely measure the changes in samples using temporally-resolved electron spectroscopy for chemical analysis (trESCA) when irradiating the samples with low-intensity, ultra-short light pulses. The new instrument, named SurfaceDynamics@FemtoSpeX, can also rapidly obtain meaningful measurements of electron energies, surface chemistry, and transient alterations using these low-intensity light pulses. Analysis of the empirical data showed that the light pulse leads to a transient accumulation of charge at the surface of the sample, triggering the phase transition at the surface from a semiconducting to a metallic state. This opens up possibilities of influencing functionality and catalytic activity in a deliberate way. *arö*

Advanced Materials (2021): Photo-driven transient picosecond top-layer semiconductor to metalic phase transition in p-doped MoS_2. N. L. A. N. Sorgenfrei, S. Neppl, R. M. Jay, D. Kühn, E. Giangrisostomi, H. Sezen, R. Ovsyannikov, S. Svensson, and A. Föhlisch. **DOI: 10.1002/adma.202006957**

"GREEN CHEMISTRY": BESSY II SHEDS LIGHT ON MECHANOCHEMICAL SYNTHESIS

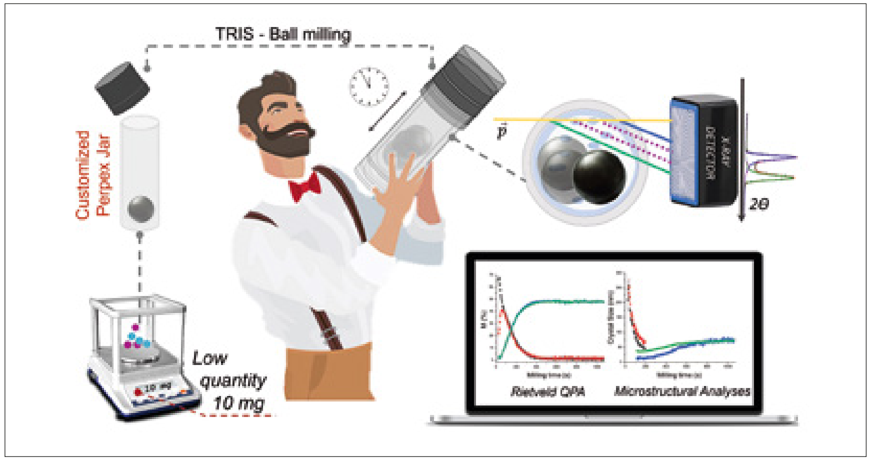
Chemical reactions are often based on the use of solvents that pollute the environment. Yet, many reactions can also work without solvent. This is the approach known as mechanochemistry, in which reagents are very finely ground and mixed together so that they react with each other to form the desired product. The mechanochemical approach is not only more environmentally friendly, but even potentially cheaper than classical synthesis methods. The International Union of Pure and Applied Chemistry (IUPAC) therefore ranks mechanochemistry among the ten chemical innovations that will change our world. However, the full potential of this technology cannot be realized until the processes during mechanical treatment are understood in more detail, so that it is possible to precisely direct and control them.

Finely ground powders can also react with each other without solvents to form the desired product. This is the approach of mechanochemistry. © F. Emmerling/BAM

Understanding what exactly happens during mechanical treatment and how the reactions take place is difficult to study. Traditionally, this is done by stopping the reaction and removing the material from the reactor for analysis "ex situ". However, many systems continue their transformation even after the milling process is stopped. Such reactions can only be studied by directly examining the reaction in situ during mechanical treatment.

Time-resolved in situ monitoring

An international team including Adam Michalchuk and Franziska Emmerling from the Federal Institute for Materials Research (BAM) and researchers at the University of Cambridge and University of Parma used BESSY II's µSpot beamline to develope a method to gain insight in situ and during mechanical treatment. To do so, the team used a combination of miniaturized grinding jars together with innovations in X-ray powder diffraction and state-of-the-art analysis strategies to significantly increase the quality of data from time-resolved in situ monitoring (TRIS).



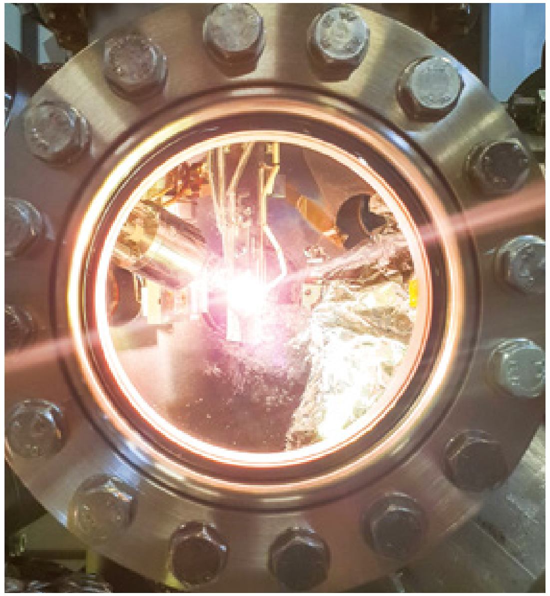
The reagents are ground in a ball mill. During this process, the formation of new products and phases can be followed via X-ray structure analysis at BESSY II. © F. Emmerling/BAM

Good results with very small samples

"Even with exceptionally small sample volumes, we get an accurate composition and structure of each phase over the course of the reaction," explains Michalchuk. Even with sample amounts as small as a few milligrams, good results were possible. In addition, they can determine the crystal size and other important parameters. This strategy is applicable to all chemical species, is easy to implement, and provides high-quality diffraction data even with a low-energy synchrotron source. "This provides a direct route to the mechanochemical study of reactions involving scarce, expensive or toxic compounds," Emmerling resumes. *arö*

Nature communications (2021): Changing the game of time resolved X-ray diffraction on the mechanochemistry playground by downsizing. Giulio I. Lampronti, Adam A. L. Michalchuk, Paolo P. Mazzeo, Ana M. Belenguer, Jeremy K. M. Sanders, Alessia Bacchi and Franziska Emmerling. **DOI: 10.1038/s41467-021-26264-1**

ULTRAFAST MAGNETISM: HEATING MAGNETS, FREEZING TIME



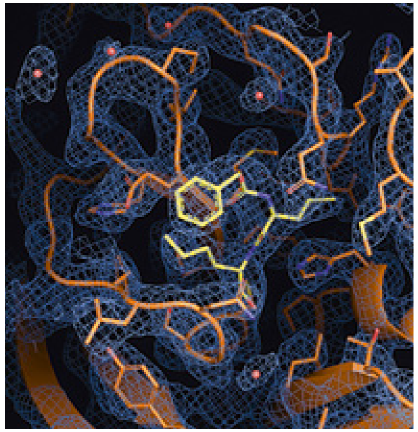
The glowing filament keeps the sample at constant temperatures during the measurements. © HZB

Magnetic solids can be demagnetised quickly with a short laser pulse, and there are already so-called HAMR (Heat Assisted Magnetic Recording) memories on the market that function according to this principle. However, the microscopic mechanisms of ultrafast demagnetisation remain unclear. A team at HZB has developed a new method at BESSY II to quantify one of these mechanisms and applied it to the rare-earth element Gadolinium, whose ferromagnetic properties are caused by electrons on both the 4f and the 5d shells. The higher the temperature, the more the crystalline sample vibrates – and as physicists say: the more the population of phonons increases, and the more likely spin-flips are to occur due to the scattering of electrons with phonons from the crystal lattice. Using the method of inelastic X-ray scattering (RIXS), the physicists were not only able to determine the number of phonons at a given temperature, but also to distinguish the interactions between phonons and 4f- and 5d-electrons. This study is completing a series of experiments done by the HZB team at BESSY II on Nickel, Iron-Nickel Alloys and now Gadolinium. Understanding these mechanisms in detail is useful for developing ultrafast data storage devices. *arö*

Applied Physics Letters (2021): Spin-lattice angular momentum transfer of localized and valence electrons in the demagnetization transient state of gadolinium. R. Decker, A. Born, K. Ruotsalainen, K. Bauer, R. Haverkamp, R. Büchner, A. Pietzsch, and A. Föhlisch. **DOI: 10.1063/5.0063404**

PROMISING CANDIDATES FOR COVID DRUGS IDENTIFIED

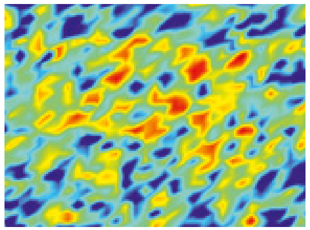
At DESY's high-brilliance X-ray light source PETRA III, a team from more than 30 research institutions has identified several candidates for active substances against the coronavirus SARS-CoV-2. They bind to an important protein of the virus and could thus be the basis for a drug against Covid-19. The MX team from HZB examined part of the measurement data with special analysis algorithms in order to identify suitable active substances. *DESY/red.*



Electron density map of the most antiviral active ingredient calpeptin (yellow) binding at the main protease. © S. Günther/DESY

Science (2021): X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Sebastian Günther, Patrick Y. A. Reinke, et al. **DOI: 10.1126/science.abf7945**

WHEN VIBRATIONS INCREASE ON COOLING



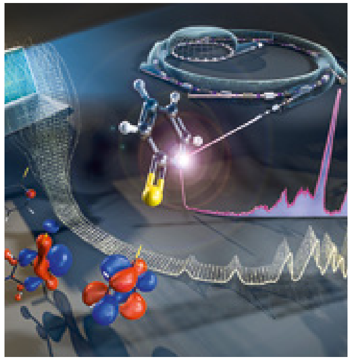
The development of this speckle pattern reveals over time microsocopic fluctuations in the material. © DOI: 10.1103/PhysRevLett.127.057001

An international team has observed an amazing phenomenon in a nickel oxide material during cooling: Instead of freezing, certain fluctuations actually increase as the temperature drops. Nickel oxide is a model system that is structurally similar to high-temperature superconductors. The experiment shows once again that the behaviour of this class of materials still holds surprises. *red.*

Phys. Rev. Lett. (2021): Measurement of Spin Dynamics in a Layered Nickelate Using X-Ray Photon Correlation Spectroscopy: Evidence for Intrinsic Destabilization of Incommensurate Stripes at Low Temperatures. A. Ricci, N. Poccia, G. Campi, C. Schüßler-Langeheine et. al. **DOI: 10.1103/PhysRevLett.127.057001**

AN EFFICIENT TOOL TO LINK X-RAY EXPERIMENTS AND AB INITIO THEORY

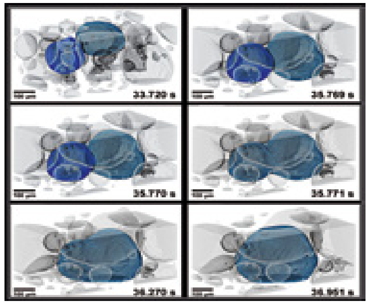
The electronic structure of complex molecules and their chemical reactivity can be assessed by the method of resonant inelastic X-ray scattering (RIXS) at BESSY II. However, the evaluation of RIXS data has so far required very long computing times. A team at BESSY II has now developed a new simulation method that greatly accelerates this evaluation. The results can even be calculated during the experiment. Guest users could use the procedure like a black box. *arö*



The electronic structure of complex molecules can be assessed by the method of resonant inelastic X-ray scattering (RIXS) at BESSY II.

© M. Künsting/HZB

Physical Chemistry Chemical Physics, issue 3 (2021): TD-DFT simulations of K-edge resonant inelastic X-ray scattering within the restricted subspace approximation. Vinícius Vaz da Cruz, Sebastian Eckert and Alexander Föhlisch. **DOI: 10.1039/D0CP04726K**



Tomographic investigation of morphology, size and cross-linking of bubbles in metal foams.

© DOI: 10.1002/adma.202104659

NEW WORLD RECORD IN X-RAY MICROSCOPY

Tomoscopy is an imaging method in which three-dimensional images of the inside of materials are calculated in rapid succession. A team led by HZB physicist Francisco García-Moreno has achieved a new world record at the Swiss Light Source at the Paul Scherrer Institute: with 1000 tomograms per second, it is now possible to non-destructively document very fast processes and developments in materials on the micrometre scale. *arö*

Advanced Materials (2021): Tomoscopy: Time-resolved tomography for dynamic processes in materials. F. García-Moreno, P. Hans Kamm, T. R. Neu, F. Bülk, M. A. Noack, M. Wegener, N. von der Eltz, C. M. Schlepütz, M. Stampanoni, J. Banhart. **DOI: 10.1002/adma.202104659**

TOMOGRAPHY BRINGS INSIGHTS INTO THE EARLY EVOLUTION OF BONES

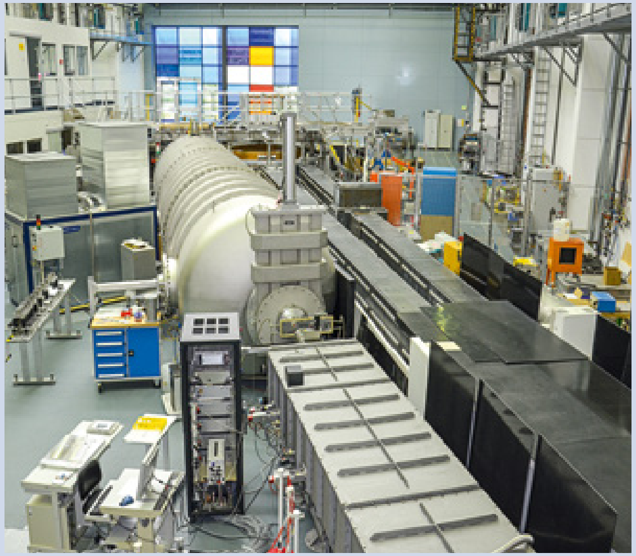
Almost all vertebrates have bones with embedded bone cells that are connected to each other via countless nanochannels. But when in the course of evolution did this complex network emerge and why has it largely prevailed? A team of palaeontologists at the Museum für Naturkunde Berlin led by Florian Witzmann has now analysed such structures in unprecedentedly high resolution for the first time in fossils of marine organisms that are around 400 million years old. One sample came from *Tremataspis mammillata*, a jawless armoured fish. The second sample was a piece of bone from the jawed armoured fish *Bothriolepis trautscholdi*. To make the structures visible, HZB expert Ingo Manke suggested a method that is available at the HZB campus in Wannsee in the Electron Microscopy Laboratory: focussed ion-beam scanning electron microscopy (FIB-SEM) tomography on the ZEISS Crossbeam 340. In this process, a focused gallium ion beam continuously removes material from the sample surface and gradually digs further into the sample – at the same time, an electron beam scans the freshly removed part of the sample and provides data for creating 3D images with a resolution that is more than a hundred times more accurate than computer tomography. *arö*

An impression of the placoderm fish living 380 million years ago. The structure of his bone cells have now been analysed in detail. .

© B. Engh/dontmesswithdinosaurs.com

Science Advances (2021): Bone Metabolism and Evolutionary Origin of Osteocytes. Y. Haridy, M. Osenberg, A. Hilger, I. Manke, D. Davesne, F. Witzmann. **DOI: 10.1126/sciadv.abb9113**

Climate-neutral: HZB strives for a climate-neutral society through science and innovation. For this reason, it is driving material discovery, creating new sustainable technologies and supporting the research community to achieve this goal. © HZB



High-quality: The instruments of the Berlin neutron source BER II, which was shut down at the end of 2019, will continue to be used in Germany and abroad. In 2021, the small-angle scattering instrument (VSANS) was transferred to the Breazeale Research Reactor at Penn State University. © A. Kubatzki/HZB

FACTS AND FIGURES ABOUT HZB

As of 31.12.2021

633

WoS, SCOPUS or Open Research Europe indexed publications were published by HZB scientists in 2021.

23.5

percent of HZB's 718 scientific staff were women at the end of 2021. In relation to the total number of 1,133 employees, the proportion of women was 31.2 percent.

182

doctoral students were supervised at HZB in 2021, with 26 dissertations completed at HZB.

79

percent of the beam time at BESSY II was used by external scientists at HZB in 2021.

314

days were dedicated to scientific use, test operation and maintenance of the storage ring facility BESSY II in 2021. It was available to users on 247 days. This corresponds to an availability of 78.7 percent. As a result of the pandemic-related travel and work restrictions as well as safety requirements in the BESSY II experimental hall, 10.5 percent of the available operating time could not be used by guest scientists.

247

cooperatives were maintained by HZB with other scientific institutions at the end of 2021 – a slight decrease compared to the previous year (270).

36

adolescents and young adults were in eight different apprenticeships at HZB at the end of 2021. The proportion of women among the trainees was 36.1 percent.

33.58

million euros in third-party funding went to HZB in 2021. This included approximately 3.29 million euros from contract research, 7.37 million euros from services to third parties, around 13.87 million euros from project funding from the federal government and about 2.15 million euros from the EU.

11

Young Investigator Groups conducted research at HZB in 2021, one more than in the previous two years. Nine of these Young Investigator Groups are part of the "Materials and Technologies for the Energy Transition" programme. Another one each is assigned to the programme part "Natural, Artificial and Cognitive Information Processing" and "From Matter to Materials and Life".

89

new collaborations with companies were established by HZB in 2021 alone. This means that the total number of ongoing partnerships with industry has increased significantly from 149 in the previous year to 205 now. Of these, almost 29 percent were collaborations with international partners and almost 18 percent were joint projects with small and medium-sized enterprises.

4.19

million euros were received by HZB for technology transfer in 2021. Of this, 1.05 million euros came from research and development partnerships and R&D orders with domestic and international commercial enterprises, and just over one million euros from other R&D cooperatives. Another 2.13 million euros originated from infrastructure agreements.

466

pupils experimented in the "Look into Matter" school laboratory from September to December 2021 after the resumption of presence operation – naturally in compliance with an appropriate hygiene concept.

8

patents were granted to HZB in 2021. HZB's patent portfolio comprised 171 patents at the end of 2021. 25 patents are the subject of ongoing licence agreements. For 23 invention disclosures from 2021, HZB and other technology experts are currently evaluating whether they can be patented and/or are commercially exploitable.

Zertifikat seit 2011
audit berufundfamilie

Family-friendly: In 2021, the HZB was awarded the "berufundfamilie" audit certificate for the fourth time for its successful promotion of a life phase conscious working culture.

© berufundfamilie Service GmbH

Ready for the Olympics: Felicia Laberer, who is completing an apprenticeship in office management at HZB, won the bronze medal in the 200-metre para-kayak single at the 2021 Paralympics in Tokyo.

© https://www.kanu.de/Athleten-74456.html

HZB Graduate Center for doctoral students

Since 2021, the HZB Graduate Center has provided all the services of the former "PhD Coordination". To this end, the services and standards at HZB for doctoral researchers and their supervisors have been gradually expanded since the beginning of 2018. The ideas and suggestions that were collected in discussions with numerous stakeholders and in various HZB committees on this topic are leading the way. The overarching goal is to create the best possible conditions for the successful completion of a doctoral thesis, while at the same time offering doctoral researchers room for individual development. An important milestone in the establishment of the umbrella structure was already reached at the beginning of 2020 with the introduction of the revised doctoral guidelines and an HZB supervision agreement. Uniform, transparent and reliable standards for all HZB doctoral researchers have been established, and support and qualification offers for them and their supervisors are being continuously expanded and developed.

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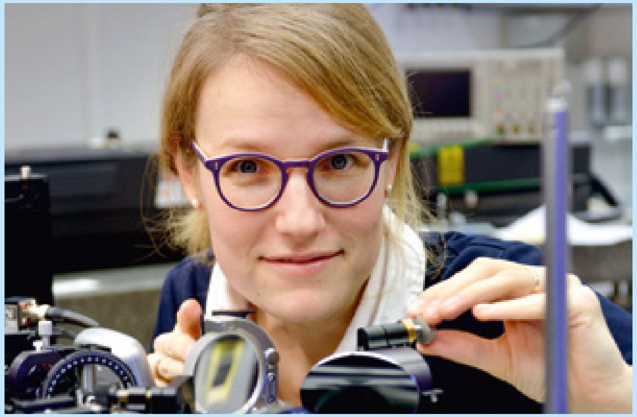
The 4000th eye tumour patient treated

For more than 20 years, Charité – Universitätsmedizin Berlin and HZB have jointly offered irradiation of eye tumours with protons. For this purpose, the HZB operates a proton accelerator, while the medical care of patients is provided by the Charité. On 19 February 2021, the 4000th eye tumour patient received irradiation with protons, performed by a joint team from HZB and Charité – Universitätsmedizin Berlin. The number of patients treated remained almost unchanged during the Corona pandemic despite the difficult conditions. The treatment in Berlin-Wannsee is only available for uveal melanomas of the eye. The proton accelerator at HZB is the only therapy site for this disease in Germany. "We congratulate the joint team on this great success and thank them for doing everything they could under the difficult pandemic conditions to maintain the operation of the life-saving eye tumour therapy," says Bernd Rech, spokesman for the scientific management of HZB.

Overview: Number of patients treated with prontons at HZB from 1998 to 2020. © S. Kodalle/HZB

New research group under development

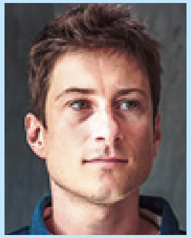
Since June 2021 Renske van der Veen is setting up the new research group "Atomic Dynamics in Light-Energy Conversion" at HZB. The chemist is an expert in time-resolved X-ray spectroscopy and electron microscopy and studies catalytic processes that enable the conversion of solar energy into chemical energy. Renske van der Veen successfully obtained a Helmholtz Funding of first-time professorial appointments of excellent women scientists (W2/W3), whereupon the HZB has already initiated an S-W2 appointment procedure at Technical University Berlin. She has 14 years of experience in the field of ultrafast X-ray methods. "At BESSY II, I can apply and expand this experience in my research project," says van der Veen.



Dr Renske van der Veen has a lot of experience with ultrafast x-ray measurements. © I. Böttcher-Gajweski/MPIBC

APPOINTMENTS, AWARDS AND PRIZES

Professor Olga Kasian has now accepted a professorship at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). The W2 professorship is entitled “Materials for Electrochemical Energy Conversion” and is located at the Faculty of Engineering.

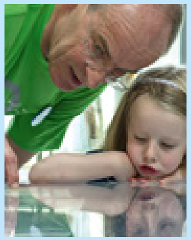


Professor Antonio Abate has accepted a W2 professorship in the Department of Chemistry at Bielefeld University. Abate investigates perovskite semiconductors for low-cost and highly efficient solar cells and heads the department “Active Materials and Interfaces for Stable Perovskite Solar Cells” at HZB.

Dr Felix Büttner has been awarded the Walter Schottky Prize for 2022 by the German Physical Society (DPG) for his pioneering achievements in the field of mag-netic skyrmions. Büttner has led a Young Investigator Group on topological solitons at HZB since 2020. According to DPG, “his work has contributed significantly to the understanding of the ultrafast generation and properties of these topological states.”

Tobias Henschel and his team have won the HZB Technology Transfer Prize 2021. Together with industry partners, the winners developed a transparent photovoltaic that was integrated into a collection of digital sport wristwatches.

Dr Fredrik Johansson from the French Institut des NanoSciences de Paris, CNRS, Sorbonne, received the Ernst Eckhard Koch Prize 2021 for his outstanding dissertation at Uppsala University on “Core-hole Clock Spectroscopy Using Hard X-rays – Exciting States in Condensed Matter”.



Dr Roland Müller received the International Conference on Accelerator and Large Experimental Physics Control Systems (ICALEPCS) Lifetime Achievement Award at a conference. In the more than thirty years of his career at BESSY, the physicist has advanced many projects on control systems at accelerators and has been particularly committed to the international exchange of knowledge.

Professor Susan Schorr and her team received a special honour on the occasion of the 10th anniversary of the Royal Society of Chemistry (RSC) journal RSC Advances: their publication on hybrid perovskite structures (DOI: 10.1039/C8RA09398A) was selected for a special anniversary compilation. The paper from HZB is considered to be one of the most important contributions to solar energy in recent years in this journal.

Professor Marianne Liebi and **Dr Manuel Guizar-Sicairos** from the Paul Scherrer Institute (PSI), Switzerland, received the Innovation Award Synchrotron Radiation 2021, which is donated by the Friends of HZB Society. Together with their teams, they developed a method to obtain information about textures in materials on the nanoscale from small-angle scattering data using mathematical methods. This method is now used at many synchrotron sources and has opened the door to fascinating studies of hierarchical structures in life and materials science.

BATTERY RESEARCH - SKALIS PROJECT FUNDED WITH 2.2 MILLION EUROS

The HZB department "Electrochemical Energy Storage" has already set up the appropriate infrastructure for SkaLis: The so-called "Pouch Cell Line", where experimental batteries can be produced in a flat "pocket format" from the starting materials lithium and sulphur in several simple steps. © HZB

Powerful, compact, and affordable batteries are needed for the energy transition. Groups at HZB led by Yan Lu, Ingo Manke, and Sebastian Risse are conducting this research. They are investigating and developing novel types of electrode materials based on sulphur and silicon. Risse is now also coordinating a large project involving teams from HZB as well as from the University of Potsdam, the Technische Universität Berlin, the Technische Universität Dresden and the Fraunhofer Institute for Material and Beam Technology IWS Dresden. The SkaLiS project has started in July 2021 and will receive a total of 2.2 million euros in funding until 2024 from the German Federal Ministry of Education and Research. SkaLiS stands for "Operando analysis-supported, trans-scale and scalable electrode design for increasing the performance of lithium-sulphur pouch cells". The participating research groups in SkaLiS intend to produce a lithium-sulphur (Li-S) demonstrator battery in pouch cell format whose cathode simultaneously exhibits structure at several scales. This approach should enable the Li-S battery to be considerably safer, offer longer service life, and higher performance than previous battery cells. For the assessment of industrial relevance, the consortium is supported by an industrial advisory board. *arö*

HZB COORDINATES DEVELOPMENT OF AGENTS AGAINST CORONA

The MX team at BESSY II specialises in analysing protein structures. This can also accelerate the development of drugs against COVID-19. © HZB

At the synchrotron light source BESSY II, which is operated by HZB, the structural analysis of macromolecules provides a fantastic tool to accelerate the development of effective substances against the SARS-CoV2 virus. The three-dimensional structure of the so-called viral main protease was determined at BESSY II for the first time at the beginning of 2020. This enzyme is indispensable for virus replication. Knowledge of this structure decisively limits the spectrum of possible substances – because such substances must fit like a key in a lock so that they can block the function of the enzyme. However, it is not sufficient to investigate only this one target. That is why several viral target proteins were addressed in the NECESSITY project, initiated by HZB researcher Christian Feiler. Together with partners from the Medical University of Innsbruck and the Czech University of Olomouc, the Berlin researchers have systematically advanced the development of drugs: In a high-throughput procedure, they will investigate more than 8,000 compounds at the MX beamlines of BESSY II and identify substances from them that could dock to the main protease of SARS-CoV-2 or to other target proteins. All compounds are either already approved for the treatment of other diseases or are in various clinical phases. *arö*

A WIKI FOR PEROVSKITE SOLAR CELL RESEARCH

Halide perovskites have huge potential for solar cells and other optoelectronic applications. Solar cells based on metal-organic perovskites achieve efficiencies of more than 25 percent, they can be produced cheaply and with minimal energy consumption, but still require improvements in terms of stability and reliability. In recent years, research on this class of materials has boomed, producing a flood of results that is almost impossible to keep track of by traditional means. Under the keyword „perovskite solar", more than 19,000 publications had already been entered in the Web of Science (as of spring 2021). Now 95 experts from more than 30 international research institutions have designed a database to systematically record findings on perovskite semiconductors. The data are prepared according to the FAIR principles, i.e. they are findable, accessible, interoperable and reusable. After reviewing the relevant literature, they have brought together more than 42,000 individual data sets, in which the data can be filtered and displayed according to various criteria such as material compositions or component type. Researchers from several teams at HZB were involved in this study which was initiated by HZB scientist Eva Unger and implemented and coordinated by her postdoc Jesper Jacobsson. The database also offers the option to easily upload new data from new peer-reviewed publications. Not only science, but also industry will benefit: The database provides an overview of the current state of knowledge, while also uncovering gaps in knowledge from which new productive research questions can arise.

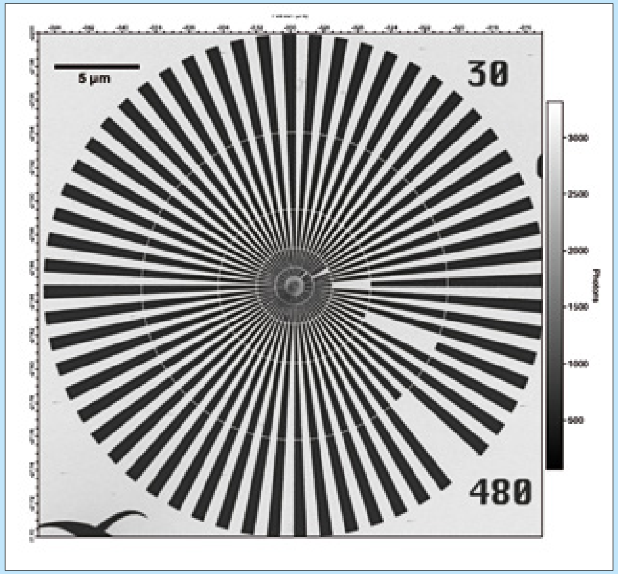
arö

Nature Energy (2021): An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles. T.J. Jacobsson, A. Hultqvist, A. García-Fernández et al. **DOI: 10.1038/s41560-021-00941-3**

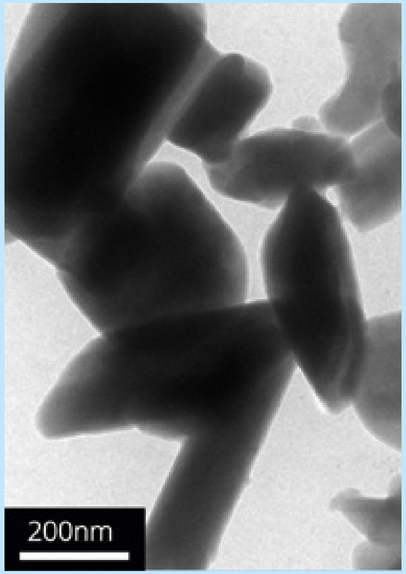
MYSTIIC AT BESSY II: NEW X-RAY MICROSCOPE PUT INTO OPERATION

A new X-ray microscope has started operation at the Energy Materials in situ Lab (EMIL). It was named MYSTIIC – Microscope for x-raY Scanning Transmission In-situ Imaging of Catalysts. With the soft X-ray light from BESSY II, it is even possible to localise individual elements and chemical compounds; the spatial resolution is below 20 nanometres. Compared to other X-ray microscopes, the STXM MYSTIIC at EMIL offers even higher precision and more options for scanning surfaces and investigating bulk samples in transmission. In particular, MYSTIIC will also allow to observe chemical processes in gas/liquid cells in the future. "It is like filming the processes taking place during catalysis," says HZB expert Markus Weigand, who is in charge of the instrument. The new microscope will thus contribute significantly to CatLab's approach on knowledge and understanding.

arö



The first image taken by MYSTIIC: a standard image use to calibrate and measure the resolution of the new STXM.
© HZB



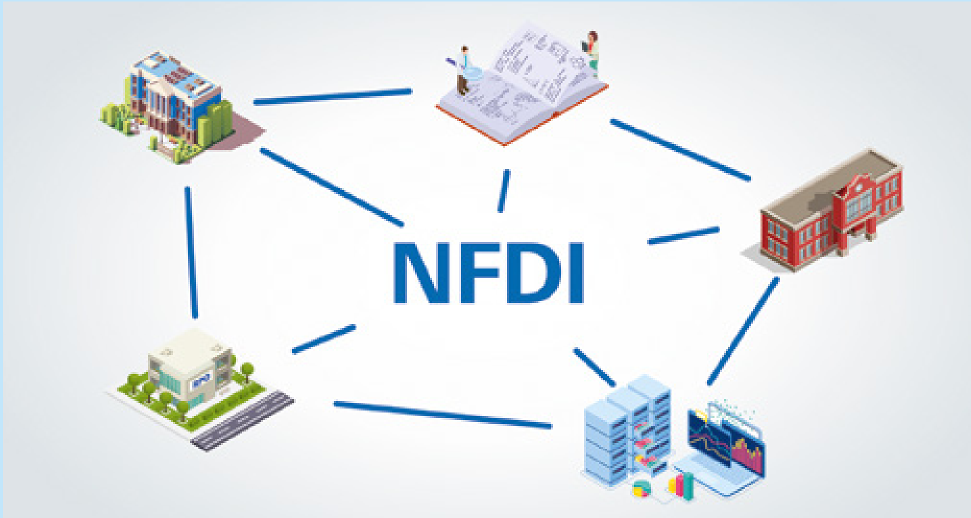
Clear microscopy image of a sample site within the transmission electron microscope (TEM). © K. Dembélé/FHI

VIPERLAB AIMS TO BOOST PEROVSKITE SOLAR INDUSTRY IN EUROPE

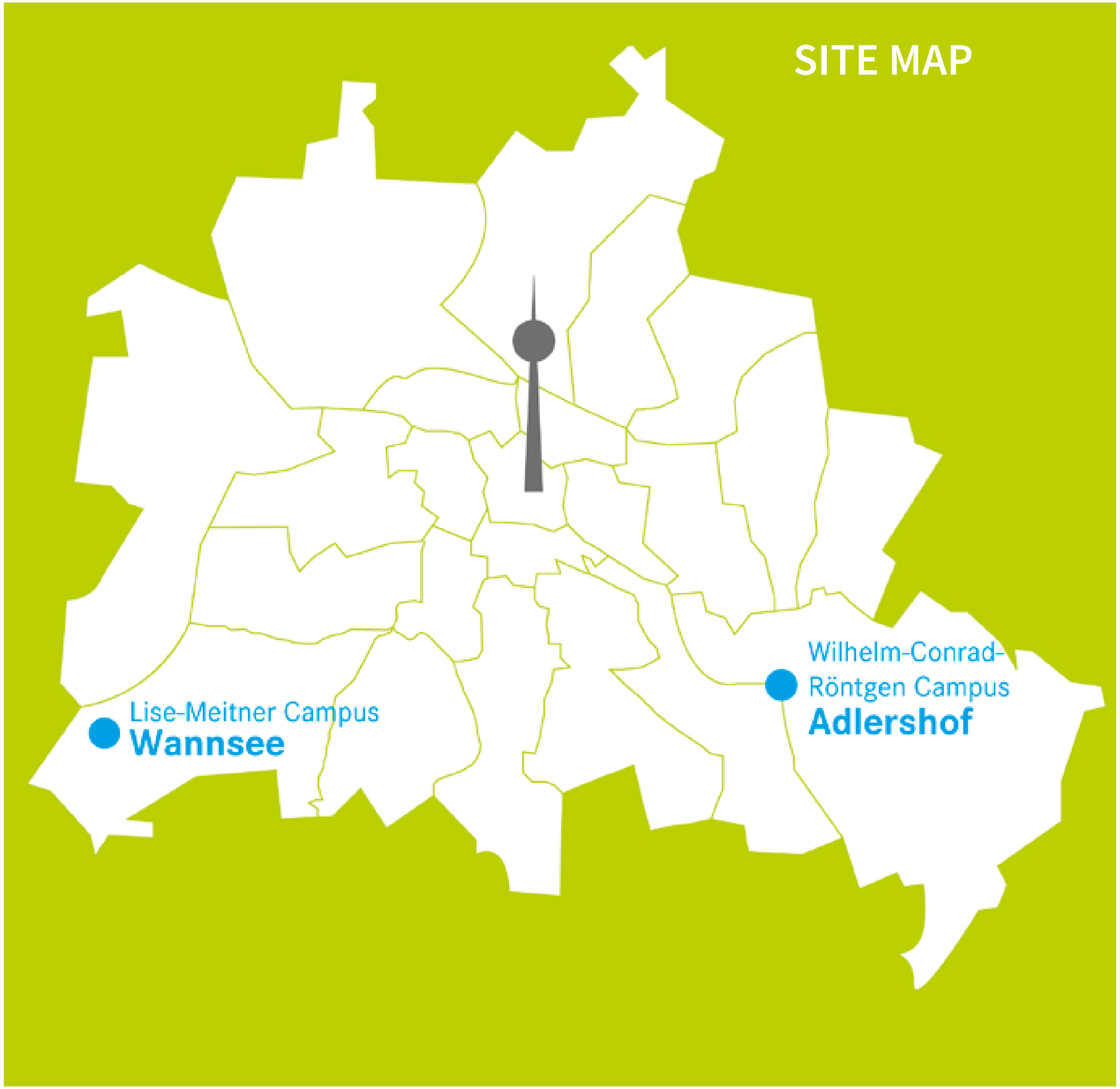
HZB runs state-of-the-art laboratories (here HySPRINT) to advance research on perovskite solar cells.

Perovskite semiconductors enable extremely cheap and powerful solar cells. Many research results on this class of materials are obtained in European laboratories. For example, working groups at HZB have already achieved several world records with perovskite solar cells (see page 11 in these Highlights). Now the HZB is coordinating a major European collaborative project to open up new opportunities for the European solar industry. The VIPERLAB project involves 15 renowned research institutions from Europe, as well as Switzerland and Great Britain. It will be funded within the framework of the EU's Horizon 2020 programme for the next three and a half years with a total of 5.5 million euros, from which the HZB will receive just under 840,000 euros. VIPERLAB stands for "Fully connected virtual and physical perovskite photovoltaics Lab". With VIPERLAB, the participating research institutions want to accelerate the development of perovskite PV technology in Europe and promote technology transfer to industry. To this end, they want to establish a close dialogue with the emerging perovskite industry in Europe, both with the help of new initiatives and with more established players such as the European solar industry association Solar Power Europe. *arö*

DAPHNE MAKES DATA FROM EXPERIMENTS SUSTAINABLY AVAILABLE



In the field of photon and neutron research, more than 28 petabytes (one petabyte is equal to one million gigabytes) of data are currently produced each year by researchers at large-scale facilities. This research data must be stored for at least ten years. Now 19 scientific institutions in Germany, among them HZB, aim to develop common standards for software, data exchange and data repositories to make research data permanently available. The DAPHNE4NFDI project (DAta from PHoton and Neutron Experiments for NFDI) will be funded over the next five years as part of the National Research Data Infrastructure and is coordinated by DESY. In research data management the FAIR criteria do apply: Data must be findable, accessible, interoperable and reusable, for humans as well as for algorithms. The connection to artificial intelligence methods or machine learning are also part of the task. HZB is contributing its expertise in research data management to the project. HZB has already participated in European projects such as PaNDATA, from which the data repository ICAT emerged, as well as in Helmholtz initiatives, which resulted in the Helmholtz Metadata Collaboration Hub matter being located at HZB. *arö*



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Dr. Ina Helms (ih, responsible), Antonia Rötger (arö, co-ordination), Silvia Zerbe (sz), E-Mail: ina.helms@helm-holtz-berlin.de, Editorial staff: Ralf Butscher (rb)

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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