HZB Helmholtz Zentrum Berlin

HIGHLIGHTS 2022

Helmholtz-Zentrum Berlin für Materialien und Energie

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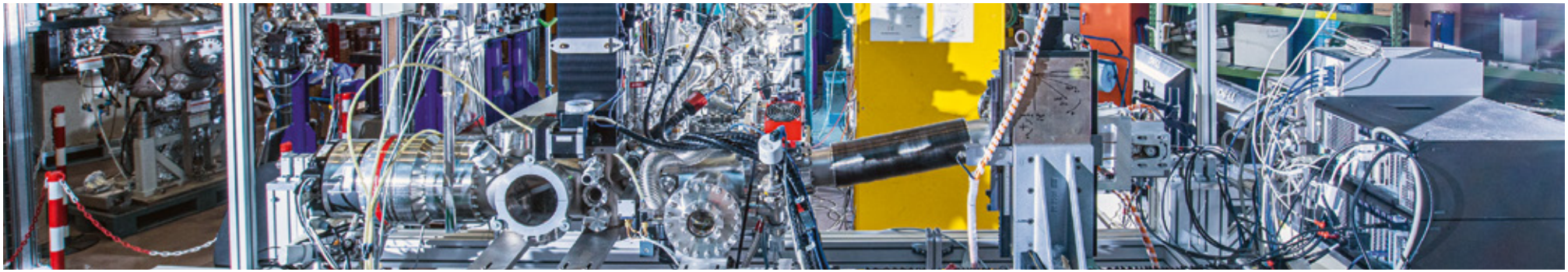

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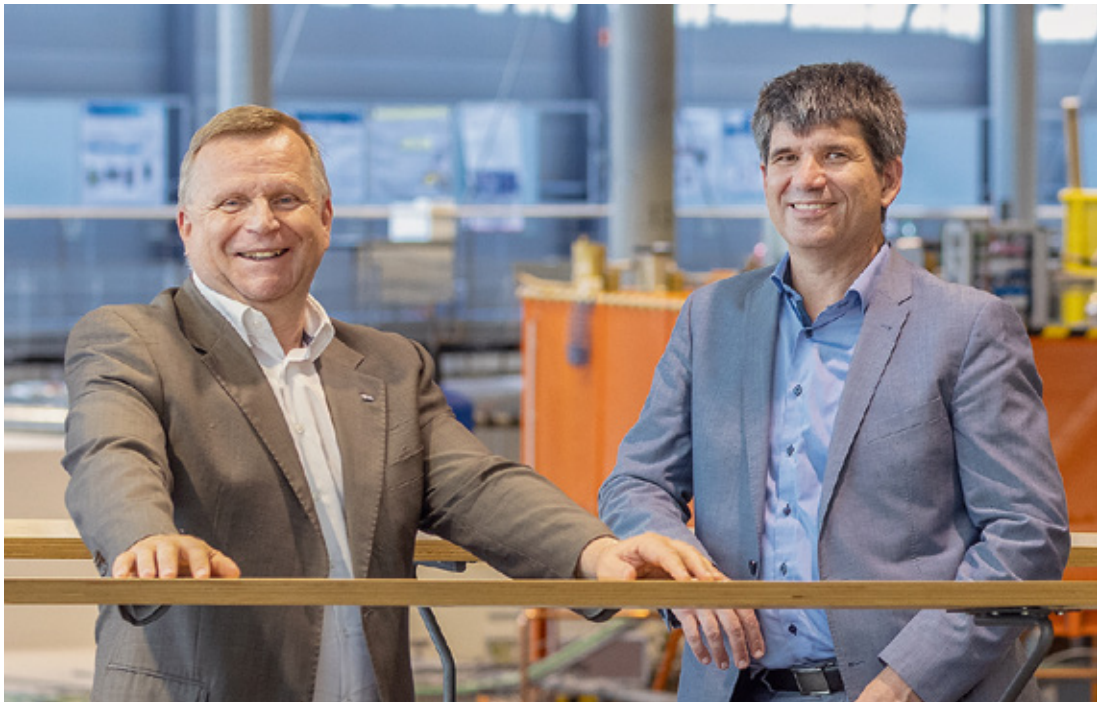
FOREWORD

In 2022, the energy supply is at the centre of public debate. Not only climate change, but also the global political situation is forcing our society to move away from oil, gas and coal more quickly than before. Renewable energy is a key technology for climate protection. But also freedom, security and prosperity depend on the success of the energy transition. Our research makes a concrete contribution. We are exploring materials that convert or store energy efficiently, we are developing next-generation solar cells, new types of batteries, quantum materials for information technology and innovative catalysts for the production of „green“ hydrogen and sustainable fuels.

And we are very successful. In 2022, for example, HZB teams once again set a world record for the efficiency of a tandem solar cell. At the same time, the experts at HZB are keeping an eye on the industry‘s requirements in terms of scaling up and costs and are working on improved manufacturing processes in close cooperation with various solar companies. Technology transfer is a central concern for us, and our research helps to strengthen the industry in Europe and the region.

In this review, we present selected research results from more than 600 scientific publications that appeared in the course of 2022. Divided into the three research areas Energy, Information and Matter, they provide an insight into the diversity of research at HZB and at our X-ray source BESSY II. The Matter section also includes exciting work by visiting scientists at BESSY II, including the analysis of biological samples in X-ray light. BESSY II is an indispensable tool for scientific progress, which we are consistently developing towards an „energy synchrotron“ – not least with the BESSY II+ extension programme proposed in 2022, which has received excellent reviews.

We recognise that science is a team effort that thrives on diversity. That is why we encourage diversity in HZB. It is an important prerequisite for creativity and an integral part of our working culture. In 2022, we signed the German Diversity Charter, in which 4,900 national and international companies publicly commit to a respectful and non-judgmental working environment. This is a further incentive for us to continue on our chosen path.



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

Bernd Rech
Scientific Managing Director

Thomas Frederking
Commercial Managing Director

“WE ARE CURRENTLY IN A DECISIVE PHASE FOR PHOTOVOLTAICS”

For the past year, HZB researcher **Rutger Schlatmann** has been Chair of the platform ETIP-PV, which brings together representatives of science, industry and politics from all over Europe. We interviewed him about the current boom – and about why the photovoltaics ship has not yet sailed for the European Union.

Rutger Schlatmann, when you specialised in photovoltaics some decades ago, it was a niche topic. Did you already have an inkling back then, that it would ever come to the boom we are experiencing today?
(With a laugh): I wish I had such clairvoyant abilities! There were some indications: for example, photovoltaics had grown continuously over the previous 20 years and it was becoming increasingly clear how important it is to avert the climate crisis. So, I was confident that the market would gain momentum in Europe. But that it would come to two such deep ruptures as the coronavirus pandemic and the war in Ukraine – I did not see those coming.

What do these crises have to do with photovoltaics – except of course for the increased demand for new energy sources?
We have glorified globalisation for a long time. Now, all of a sudden, we recognise that we, in Europe, can’t even produce as simple an item as a face mask without relying on a supply chain that extends all the way back into the Far East. And of course that applies even more to complex products such as medicines, semiconductor chips and, indeed, solar cells.

That would be the geostrategic perspective. What is the technological outlook on photovoltaics today?
Back when I got into research, practically nobody took the field seriously. But, for a number of years now, solar electricity has had the lowest production costs – it is more economical than electricity from oil or gas and, as probably goes without saying, it is much cheaper than nuclear energy. And there is still enormous potential for further advancements in the technology. We are currently in a decisive phase for photovoltaics, and the good news is: the research landscape in Europe, and in Germany especially, has become much stronger and larger than one might have expected given the industrial capacities that still exist in this field here in Germany.

But we are seeing strong output from photovoltaics researchers in China as well, aren’t we?
Most definitely, and we should not underestimate that in terms of quantity or quality. But we’re in the lead for certain technologies that are currently in very high demand because Germany has been investing a lot of research funding into them over the past ten years. Perovskite tandem solar cells are a good example: these have two overlaid layers, a silicon layer and a perovskite layer, each of which converts different colour components of sunlight into energy, and that makes them work at much higher efficiency than conventional solar cells. There’s been incredible progress in their efficiency, but also in their stability. At HZB alone, we have recruited several groups and talents dedicated to this technology. And it’s like that not only in research, by the way, but also in the commercial sector.

“The research landscape in Europe, and in Germany especially, has become much stronger and larger than one might have expected given the industrial capacities that still exist in this field here in Germany.”

That brings me to the next question. About a year ago, you entered office as the Chair of the European Technology and Innovation Platform for Photovoltaics. What new things have you learned since then?

More than anything, I have gained deeper insights into the regulatory and political conditions. An awful lot has started moving in this field. The dominant topic is of course the Inflation Reduction Act of the US, a humungous programme aimed at supporting the establishment of production capacities. The investment opportunities are so attractive that, when talking with companies these days, I keep hearing that they would actually like to invest in Europe, but that the differences are so great that they're in fact better off producing in the US and then shipping the goods to Europe from there.

Couldn't we, in Europe, just skip the traditional silicon solar cell phase and go straight on to scaling up production of tandem technology?

No, there are two reasons why that won't work. The first is that the ship has not yet sailed for silicon cells; quite the opposite. And, secondly, we first have to build the entire value creation chain in Europe back up from scratch – and for silicon technology that would be okay. The solar companies need extremely transparent glass, for example. Companies that can produce such a thing do exist in Europe, but they shut this segment down a long time ago because there was no demand. And the same goes for so many other components you need to manufacture PV modules. Luckily, the knowhow for all those things still exists – but production has to be ramped up again first.

"The incredible progress in photovoltaics at HZB is not only noticed in research, but also in the commercial sector."

So, are the necessary steps actually being taken towards this?

It never ceases to amaze me how politics works in the EU – how some countries can block a sensible bill, for example, just so that they can get more for themselves out of the negotiations. Although, I can imagine that the European Commission, as well as the national governments, are well aware of how great the pressure to act is. Yet there are also rays of hope: in battery production, for example, an investment climate has set in that has made Europe attractive again for an industry that had in fact long since migrated away.

Would you say you are more optimistic or more pessimistic about the PV industry, now that you have had several chances to look behind the scenes from your new office?

Without a doubt: I am more optimistic.

Interviewed by Kilian Kirchgessner.

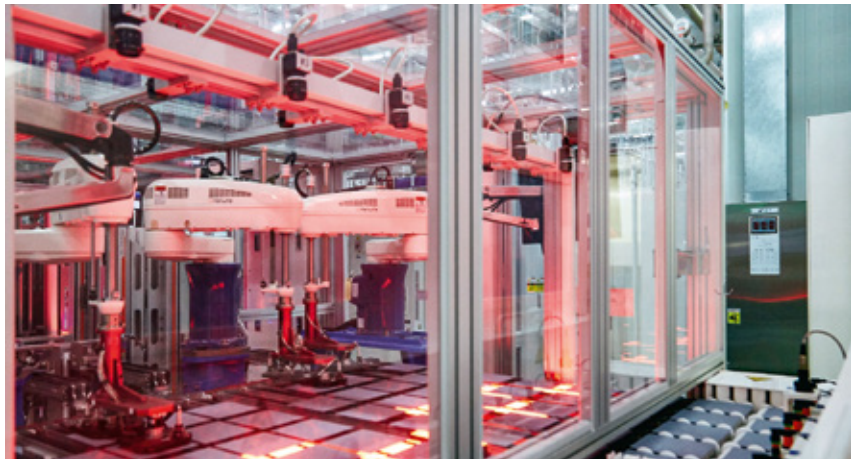
Short biography

Professor Rutger Schlatmann heads the Competence Centre Photovoltaics Berlin (PVcomB) at Helmholtz-Zentrum Berlin and teaches as a professor at HTW Berlin University of Applied Sciences. Since October 2022, he has been the Chair of the European Technology and Innovation Platform for Photovoltaics (ETIP PV). Research institutes, industrial companies and political figures have joined together in this advisory body of the European Commission. The Dutch professor studied physics in Groningen and Amsterdam and worked for many years in responsible positions in industrial research before coming to HZB in 2008.

EUROPEAN PILOT LINE FOR INNOVATIVE TANDEM SOLAR CELLS

PEPPERONI is a four-year Research and Innovation project co-funded under Horizon Europe and jointly coordinated by Helmholtz-Zentrum Berlin and Qcells. The project will help advance perovskite/silicon tandem photovoltaics (PV) technology's journey towards market introduction and mass manufacturing.

PEPPERONI's goal is to identify and address the barriers to tandem solar technology's market introduction, and ultimately lay the foundations for new production capacity in Europe. The project began on 1 November 2022, with the long-term vision of enabling European industrial leadership on PV production in the global market. Under PEPPERONI, an industrial-type tandem cell pilot line will be established at Qcells' European headquarters in Thalheim, Germany, comprising innovative equipment, processes and materials for the production of high-efficiency tandem cells and modules.



View of a production line for solar cells at Qcells. ©Qcells

The project aims to achieve a fast and cost-competitive route to mass production of PV modules with high performance and long durability. It has selected technology that promises the best ratio of performance over manufacturing costs – silicon/perovskite tandem. Perovskite, a novel class material with a special crystal structure, can be fine-tuned to take advantage of the parts of the solar spectrum that typical silicon PV materials cannot utilise very efficiently, meaning they make excellent hybrid-tandem partners. "This research promises to break new ground in the advancement of perovskite-silicon tandem solar cell and module technology," says Fabian Fertig, Director Global R&D Wafer & Cells at Qcells. "At a time of unprecedented pressures on the current energy system, it is exciting to realise this first and transformative step towards industrial-scale manufacturing of next-generation PV technology in Europe."

The PEPPERONI consortium aims to tackle the challenges currently hindering the deployment of tandem solar cells and has set itself a lot of goals. For example, the minimisation of scaling losses is to be achieved thanks to innovations in the materials and equipment used. In addition to the development of processes and equipment for thin-film deposition, the operational stability of perovskites is also to be expanded through in-depth analyses of performance losses. Furthermore, the aim is to eliminate risks to human health and the environment.

PEPPERONI proposes to use a type of silicon bottom cell, which is based on already globally available technology at a gigawatt scale: Q.ANTUM technology. In addition to promising higher module efficiencies, the deposition of a perovskite top cell onto silicon bottom cells in only a few extra process steps also allows for cost-effective production scale up. "At HZB we have developed the tandem technology to world-record efficiency level on lab scale," explains Bernd Stannowski, head of group Industry compatible processes, solar cells and modules at HZB. "We are now looking forward to cooperate in the consortium with partners from science and industry to jointly scale up this new and very promising technology and transfer it to industry." *Qcells/red.*

FROM LABORATORY TO INDUSTRIAL PRODUCTION

In order to transfer tandem solar cells from laboratory scale to production, HZB is cooperating with the solar module manufacturer Meyer Burger, which has great expertise in heterojunction technology (HJT) for silicon modules, as well as other research partners. Within the framework of this cooperation, **mass production-ready silicon bottom cells** based on heterojunction technology are to be combined with a top cell based on perovskite technology.

The cluster facility operated at HZB allows to produce large-area perovskite/silicon tandem solar cells. This facility, the only one of its kind in the world, helps to develop new industry-related processes, materials and solar cells.
© B. Stannowski/HZB

For the development of next-generation, high-performance solar cells and modules, the HZB is working with Meyer Burger Technology AG. The Swiss company also cooperates with CSEM from Switzerland, the Fraunhofer Institute for Solar Energy Systems ISE in Freiburg and the Institute for Photovoltaics at the University of Stuttgart. The aim is to industrialise the perovskite tandem technology, which is expected to allow the industrial production of solar cells with efficiencies in excess of 30 percent in the future.

Meyer Burger is a manufacturer of high-quality solar modules based on silicon heterojunction technology (HJT). Meyer Burger's research and development team has already developed HJT cells in recent years together with Bernd Stannowski's team at the Helmholtz-Zentrum Berlin because HZB has great expertise in the field of perovskite solar cells. Recently, laboratory tandem solar cells combining heterojunction and perovskite have achieved record efficiencies of over 32 percent, largely due to the work of Steve Albrecht's group.

Research brings jobs to Europe

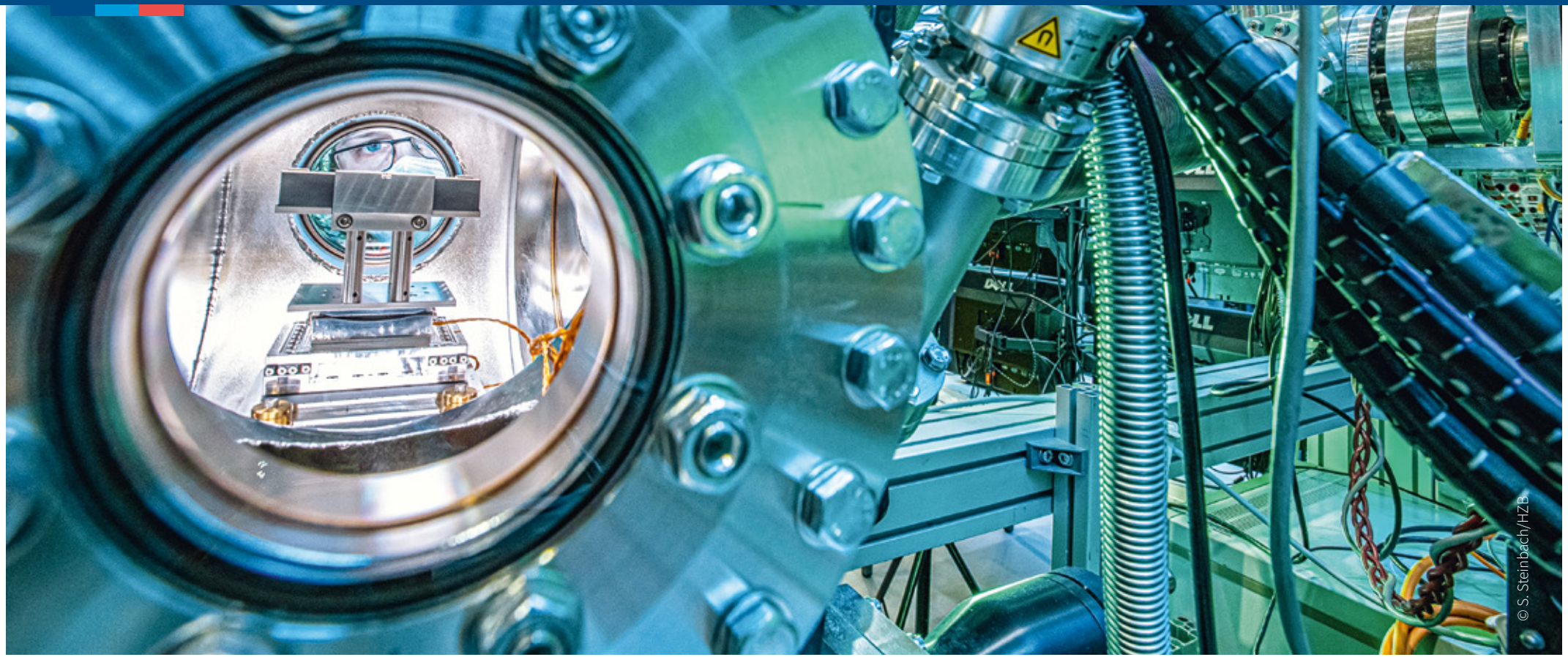
However, such record-breaking tandem cells have only the laboratory-standard areas of one square centimeter and are partly produced with processes that are not scalable. "We are therefore delighted to be cooperating with Meyer Burger to transfer this fantastic technology into application," says Stannowski, who heads the cooperation at HZB. A new cluster facility (KOALA) will also be used. This globally unique facility, funded by the German Federal Ministry of Economics and Climate Protection (BMWK) and the Federal Ministry of Education and Research (BMBF), makes it possible to produce perovskite/silicon tandem solar cells in vacuum on industry-standard large wafers.

"With a long tradition of proprietary development, Meyer Burger has an extensive portfolio of processes, technologies, and production techniques at its disposal for the potential mass production of tandem solar cells and modules in-house," says Marcel König, Head of Research and Development at Meyer Burger. "This includes the essential manufacturing processes and machinery for silicon-based perovskite tandem solar cells, as well as corresponding solar modules with Meyer Burger's proprietary SmartWire connection technology. In conjunction with the skills of our academic partners, this is a unique recipe for success." The work with the new consortium is based on existing collaborations for the development of heterojunction silicon solar cells.

"Meyer Burger manufactures in Europe and thus creates high-quality jobs. In doing so, the company is exploiting technologies that were developed in Europe," says Rutger Schlatmann, director of the Photovoltaics Competence Centre Berlin (PVcomB) at HZB. The new cooperation agreement is set to run for three years. *red.*

HIGHLIGHTS FROM RESEARCH – ENERGY

The Helmholtz-Zentrum Berlin has a leading international position in photovoltaics research, but also makes important contributions in the field of chemical energy conversion and storage. The basis for this is the work of the scientists in the various laboratories and measuring stations at BESSY II. The spectrum ranges from battery research to the development of catalytically active materials for the production of green hydrogen or the conversion of CO_2. **There is a scientific publication for almost every article. Click on this symbol for it:**



NEW WORLD RECORD FOR TANDEM SOLAR CELLS

The current world record of tandem solar cells consisting of a silicon bottom cell and a perovskite top cell is once again at HZB. The new tandem solar cell converts 32.5 percent of the incident solar radiation into electrical energy. The certifying institute European Solar Test Installation (ESTI) in Italy measured the tandem cell and officially confirmed this value which is also included in the NREL chart of solar cell technologies, maintained by the National Renewable Energy Lab, USA. “This is a really big leap forward that we didn’t foresee a few months ago. All the teams involved at HZB, especially the PV Competence Center (PVComB) and the HySPRINT Innovation lab teams have worked together successfully and with passion,” says Steve Albrecht, who leads a large team at HZB on perovskite solar cells.

Fascinating tandem technology

His team used an advanced perovskite composition with a very smart interface modification. The lead authors, postdocs Silvia Mariotti, and Eike Köhnen in Albrecht’s team, developed an interface modification to reduce charge carrier recombination losses and applied detailed analysis to understand the specific properties of the interface modification. These developments were then successfully implemented in tandem solar cells, and with help of Master’s student Lea Zimmermann, combined with further optical improvements.

In addition, many more scientists and technicians helped to develop and fabricate the tandem cells to achieve this success. Altogether, the interface and optical modifications enabled highest photovoltages (open-circuit voltage) and resulted in the new record efficiency for this fascinating tandem technology.

International race for efficiency

There is an ongoing efficiency development by various research institutes and companies in the photovoltaics industry over the last years which is quite exciting: Various teams from HZB had achieved a record value in late 2021 with an efficiency of 29.8 percent that was realised by periodic nanotextures. More recently, in summer 2022, the Ecole Polytechnique Fédérale de Lausanne, Switzerland, first reported a certified tandem cell above the 30 percent barrier.

With the new certified value of 32.5 percent, the record is again back at HZB. “We are very excited about the new value as it shows that the perovskite/silicon tandem technology is highly promising for contributing to a sustainable energy supply,” says Albrecht.

HZB’s scientific director, Bernd Rech, emphasises: “At 32.5 percent, the solar cell efficiency of the HZB tandems is now in ranges previously only achieved by expensive III/V semiconductors.” This has enabled researchers in Europe to achieve spectacular improvements over the past two years.

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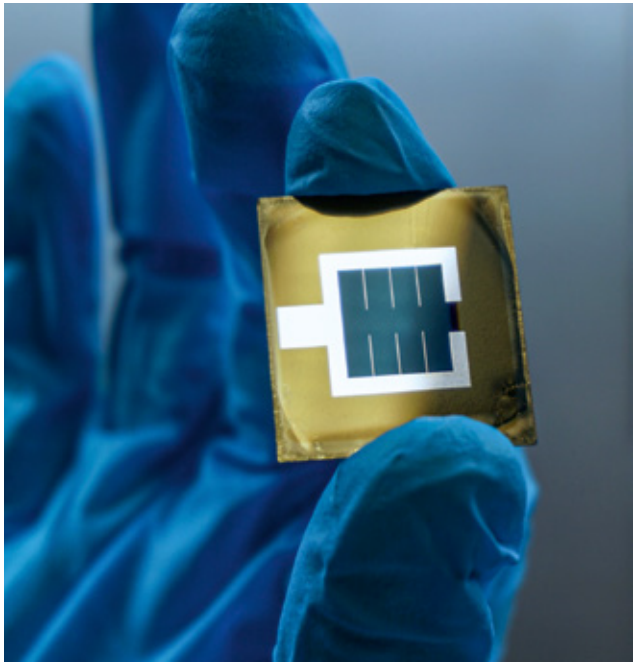
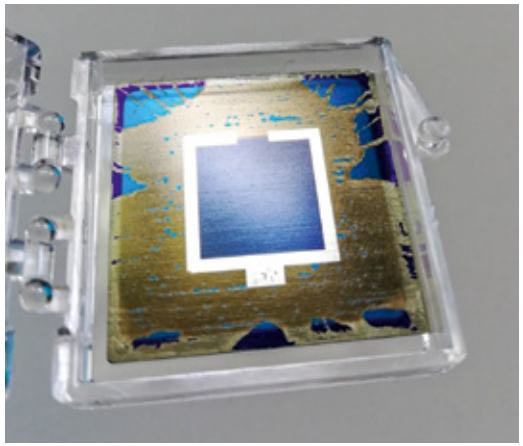


Photo of the perovskite/silicon tandem solar cell. You can see the active bluish area in the middle of the wafer, which is enclosed by the metallic, silvery electrode.

Publication on the previous “world 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**

STANDARD SILICON SOLAR CELLS COMBINED WITH PEROVSKITE TO FORM TANDEM



The HZB team has applied a perovskite top cell to a standard silicon cell. This tandem solar cell could achieve high efficiencies with further optimization.

© S. Mariotti/HZB

Tandem cells made of silicon and perovskite are able to convert the broad energy spectrum of sunlight into electrical energy more efficiently than the respective single cells. For the first time, two teams from HZB and the Institute for Solar Energy Research in Hamelin (ISFH) have succeeded in combining a perovskite top cell with a so-called PERC/POLO silicon cell to form a tandem device. This is an important achievement, since PERC silicon cells on p-type silicon are the "workhorse" of photovoltaics, with a market share of about 50 percent of all solar cells produced worldwide. They are largely optimized, temperature and long-term stable and thus ideal for the commercialization of a perovskite-silicon tandem technology.

The first perovskite PERC/POLO tandem cells produced in this way achieved an efficiency of 21.3 percent on an active cell area of about one square centimeter which is below the efficiency of optimized PERC cells. "However, initial experimental results and optical simulations indicate that we can significantly improve the performance through process and layer optimization," explains Lars Korte, the corresponding author of the study. The experts estimate a possible efficiency of 29.5 percent.

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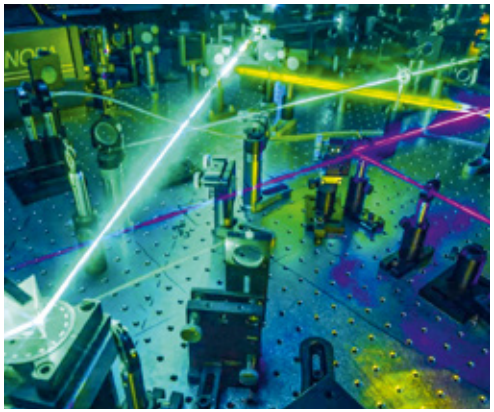
Solar – RRL (2022): Monolithic Perovskite/Silicon Tandem Solar Cells fabricated using industrial p-type POLO/PERC Silicon Bottom Cell Technology. S. Mariotti, K. Jäger, M. Diederich, M. S. Härtel, B. Li, K. Sveinbjörnsson, S. Kajari-Schröder, R. Peibst, S. Albrecht, L. Korte, T. Wietler. **DOI: 10.1002/solr.202101066**

PREDICTING SOLAR CELL PERFORMANCE FROM TERAHERTZ AND MICROWAVE SPECTROSCOPY

Many different semiconductor materials come into question for solar cells. Now a study shows how terahertz (TRTS) and microwave spectroscopy (TRMC) can be used to determine two important material properties of a semiconductor to be used as a solar cell much more precisely: the mobility and the lifetime of the charge carriers. From this measurement data, it is possible to predict the potential efficiency of the solar cell and to classify the losses in the finished cell.

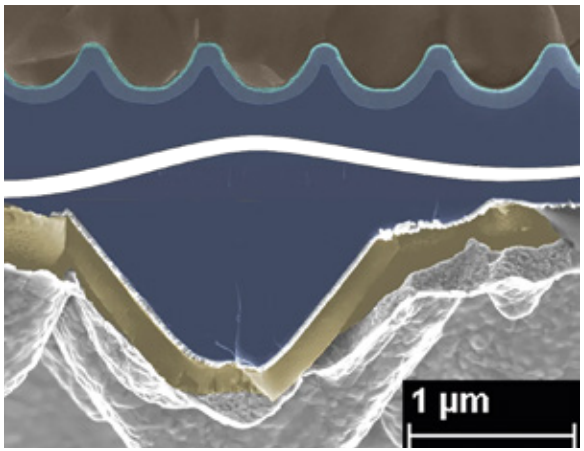


In the femtosecond laser laboratory, charge transport in semiconductors can be studied with terahertz and microwave spectroscopy. For this purpose, laser pulses first generate charge carriers in the material, which then absorb long-wave radiation (terahertz or microwaves) proportional to their mobility. © HZB

However, measurement data found in literature often differ by orders of magnitude. This has made it difficult to use them for reliable assessments of material quality. "We wanted to get to the bottom of these differences," says Hannes Hempel from the HZB team led by Thomas Unold. Therefore they contacted experts from a total of 15 international laboratories to analyze typical sources of error and problems with the measurements. "We believe that this analysis is of great interest for photovoltaic research, because it predicts the maximum possible efficiency of the material in a solar cell and reveals the influence of various loss mechanisms, such as transport barriers," says Unold. This applies also to other new semiconducting materials. *arö*

Advanced Energy Materials (2022): Predicting Solar cell performance from Terahertz and Microwave Spectroscopy. H. Hempel, T. J. Savenjie, M. Stolterfoht, J. Neu, M. Failla, V. C. Paingad, P. Kužel, E. J. Heilweil, J. A. Spies, M. Schleuning, J. Zhao, D. Friedrich, K. Schwarzburg, L. D. A. Siebbeles, P. Dörflinger, V. Dyakonov, R. Katoh, M. J. Hong, J. G. Labram, M. Monti, E. Butler-Caddle, J. Lloyd-Hughes, M. M. Taheri, J. B. Baxter, T. J. Magnanelli, S. Luo, J. M. Cardon, S. Ardo, and T. Unold. **DOI: 10.1002/aenm.202102776**

TANDEM SOLAR CELLS WITH PEROVSKITE: NANOSTRUCTURES HELP IN MANY WAYS



Scanning electron microscopy of perovskite silicon tandem cells in cross-section with nanotexture and back-reflector layer (golden). © P. Tockhorn/HZB

By the end of 2021, three teams at HZB had presented perovskite silicon tandem solar cells with an efficiency close to 30 percent. This value was a world record for eight months, a long time for this hotly contested field of research. They achieved this temporary record with nano-optical structuring and reflective coatings. “Our competences complement each other very well,” says Christiane Becker, who developed the world record cell with the team led by Bernd Stannowski (silicon bottom cell) and Steve Albrecht (perovskite top cell). Becker's team introduced a nano-optical structure into the tandem cell: a gently corrugated nanotexture on the silicon surface. “Most surprising, this texture brings several advantages at once,” emphasizes Becker: “It reduces reflection losses and ensures a more regular perovskite film formation.” In addition, a dielectric buffer layer on the back of the silicon reduces parasitic absorption at near-infrared wavelengths. As a conclusion, the researchers hold: customized nanotextures can help to improve perowskite semiconductor materials on diverse levels. These results are not only valuable for tandem solar cells made of perovskite and silicon, but also for perovskite-based light-emitting diodes.

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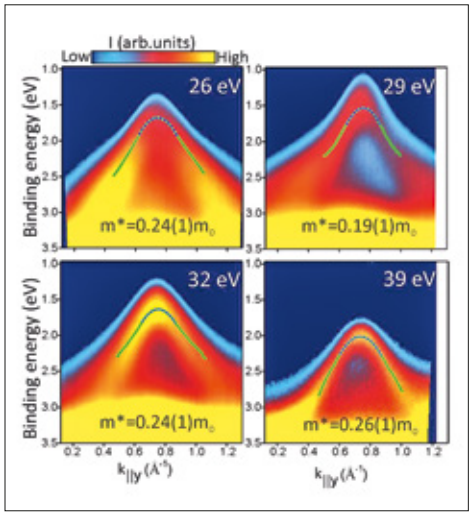
Nature Nanotechnology (2022): Nano-optical designs for high efficiency monolithic perovskite-silicon tandem solar cells. Tockhorn, J. Sutter, A. Cruz, P. Wagner, K. Jäger, D. Yoo, F. Lang, M. Grischek, B. Li, J. Li, O. Shargaieva, E. Unger, A. Al-Ashouri, E. Köhnen, M. Stolterfoht, D. Neher, R. Schlatmann, B. Rech, B. Stannowski, S. Albrecht, C. Becker. **DOI: 10.1038/s41565-022-01228-8**

PEROVSKITE SOLAR CELLS: PROPERTIES STILL REMAIN ENIGMATIC

In order to explain the particularly favourable properties of perovskite semiconductors for solar cells, various hypotheses are circulating. One assumes that polarons form in lead halide perovskites, which contribute to charge transport. Such polarons are oscillations of ions in the crystal lattice that react to the movement of electrons because of their charge. Since perovskites consist of negative (here lead) and positive ions (here caesium), the assumption that polarons play a role was obvious. With the help of measurements with angle-resolved photoemission spectroscopy (ARPES) at BESSY II, Maryam Sajedi from Oliver Rader's team was able to disprove the thesis of large polarons.



ARPES data for different photoenergies (along a certain direction of the reciprocal lattice). They show: The effective mass increases little. © HZB

A second hypothesis suspects a gigantic Rashba effect, which should limit the losses due to recombination of charge carriers. The Rashba effect is based on a strong spin-orbit coupling, which could be generated in lead-halide perovskites by the heavy metal lead. Sajedi studied several samples with spin ARPES. “This effect is at least a hundred times smaller than assumed,” she comments on the result of her analysis. “We have thus been able to experimentally disprove two common hypotheses about the transport properties in perovskites,” says Oliver Rader. This is important in order to be able to use the right levers when optimizing these materials.

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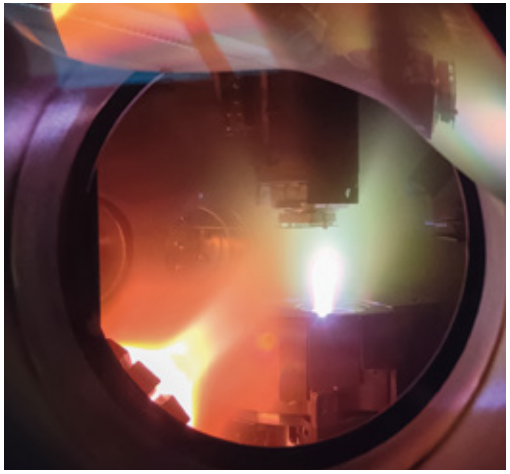
Phys. Rev. Lett. (2022): Is There a Polaron Signature in Angle-Resolved Photoemission of $CsPbBr_3$? M. Sajedi, M. Krivenkov, D. Marchenko, J. Sánchez-Barriga, A. K. Chandran, A. Varykhalov, E. D. L. Rienks, I. Aguilera, S. Blügel, and O. Rader.. **DOI: 10.1103/PhysRevLett.128.176405**

SOLAR HYDROGEN: BETTER PHOTOELECTRODES THROUGH FLASH HEATING

Photoelectrodes are needed to split water electrolytically with sunlight. Several teams at the HZB Institute for Solar Fuels are working on their development. Low-cost metal-oxide thin films with high electronic quality are very suitable for this purpose, but their production is complex. In particular, the quality of the metal oxide thin films can only be improved by thermal treatment at very high temperatures. However, this would melt the underlying conductive glass substrate.



Pulsed laser deposition: An intense laser pulse hits a target containing the material, tranforming it into a plasma which is then deposited as a thin film onto a substrate.

© R. Gottesman/HZB

A team at HZB-Institute for Solar Fuels lead by Ronen Gottesman has solved this dilemma: After deposition, using high-powered lamps, he flash-heats the metal-oxide thin film. This heats it up to 850 degrees Celsius without melting the underlying glass substrate. “The heat efficiently reduces structural defects, trap states, grain boundaries, and phase impurities, which would become more challenging to mitigate with an increasing number of elements in the metal-oxides,” says Gottesman. His team has demonstrated this on photoelectrodes made of Ta_2O_5, TiO_2 and WO_3, which were heated to 850 degrees Celsius without damaging the substrates. The new method was also successful with a photoelectrode material that is considered a very good candidate for solar water splitting: α-$SnWO_4$. Here, a performance increase of 25 percent could be achieved compared to the previous record.

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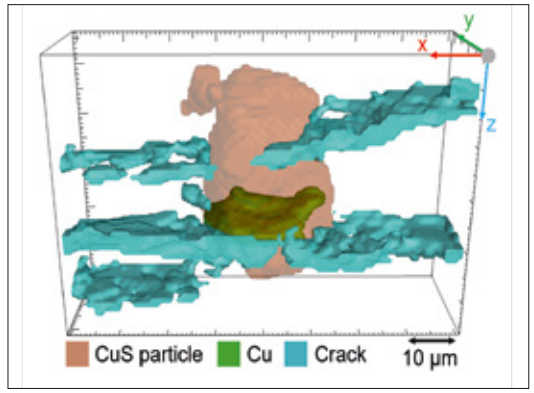
ACS Energy Letters (2022): Shining a Hot Light on Emerging Photoabsorber Materials: The Power of Rapid Radiative Heating in Developing Oxide Thin-Film Photoelectrodes. R. Gottesman, I. Peracchi, J. L. Gerke, R. Irani, F. F. Abdi, and R. van de Krol. **DOI: 10.1021/acsenergylett.1c02220**

TOMOGRAPHY SHOWS HIGH POTENTIAL OF COPPER SULFIDE SOLID-STATE BATTERIES

Solid-state batteries (SSBs) are currently regarded as a promising battery technology of the future. Compared to the current lithium-ion batteries, which are used in mobile phones, laptops and electric vehicles, SSBs could achieve even higher energy densities and better safety. Researchers from the Helmholtz-Zentrum Berlin and Hereon, Humboldt-Universität zu Berlin and the Federal Institute for Materials Research and Testing have now succeeded in observing the processes within such a solid-state battery during charging and discharging.



3D reconstruction of the formation of a copper crystallite in a copper sulfide particle (CuS) during the discharge of a lithium CuS solid-state battery. The volume expansion can lead to the formation of cracks (blue).

© K. Dong / HZB

The teams led by Philipp Adelhelm and Ingo Manke investigated the behavior of copper sulfide, a naturally occurring mineral, as a cathode in a solid-state battery. Lithium was used as an anode. A special feature of the battery is that large copper crystallites form during discharge. With the help of X-ray tomography, the formation of these crystallites could be studied in detail. Thus, the (dis)charge reaction could be traced in 3D and for the first time the movement of the cathode particles within the battery could be tracked. In addition, it was shown that cracking can be effectively reduced by higher pressure. “The results provide detailed insights into the inner workings of a solid-state battery and show how its properties can be improved,” explain Zhenggang Zhang and Kang Dong, the joint first authors of the publication.

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Advanced Energy Materials (2022): Phase Transformation and Microstructural Evolution of CuS Electrodes in Solid-State Batteries Probed by in-situ 3D X-ray Tomography. Z. Zhang, K. Dong, K. A. Mazzio, A. Hilger, H. Markötter, F. Wilde, T. Heinemann, I. Manke, P. Adelhelm. **DOI: 10.1002/aenm.202203143**

LITHIUM-SULFUR BATTERIES: FIRST MULTIMODAL ANALYSIS IN POUCH CELL FORMAT

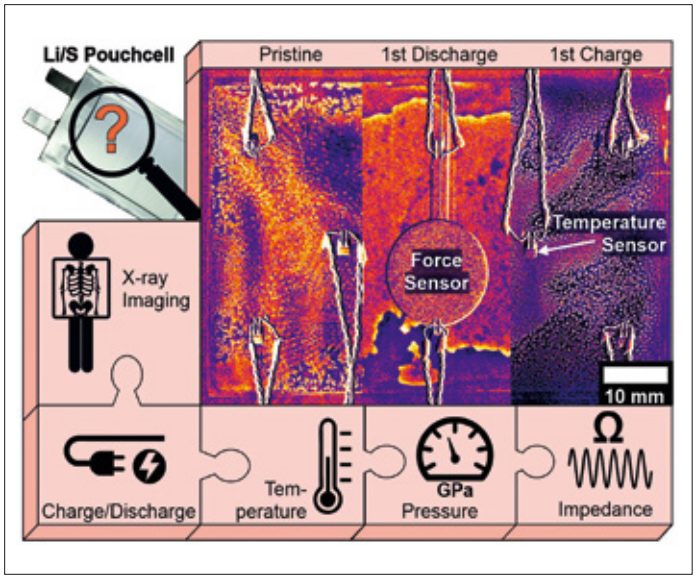
Lithium-sulphur (Li/S) batteries theoretically have an energy density of 2500 watt-hours/kg, which is significantly higher than in conventional lithium-ion batteries. In addition, Li/S batteries use more environmentally friendly cathode materials. However, with the number of charging cycles, the active material changes, the metallic lithium anode corrodes and the capacity decreases rapidly. With innovative electrolytes and refined additives, attempts are being made to slow down this ageing. So far, however, mainly Li/S batteries in coin cell design have been investigated, where these reactions take place soaked in plenty of electrolyte.

For industry, however, other formats such as round cells, prismatic cells or pouch cells are of particular interest. In these formats, the amount of electrolyte is extremely small, which enables particularly high energy densities. At HZB, multimodal operando investigations on Li/S pouch cells have now been carried out for the first time as part of the project “HiPoLiS” which is funded by the German Federal Ministry of Education and Research. In collaboration with teams from the Technical University Dresden as well as the Fraunhofer Institute for Material and Beam Technology IWS, a team led by Sebastian Risse investigated single-layer Li/S cells with different electrolytes. “We first need to understand the processes in monolayer cells before we can also optimise multiple layers in pouch cells,” Risse points out.

Radiography and sensors combined

For their study, they combined measurement data with X-ray radiography analyses, which were created in close cooperation with the group led by HZB imaging expert Ingo Manke. “This allowed us to draw conclusions about the formation and deposition of sulphur particles and polysulfides over the course of the charging cycles,” says Rafael Müller, a postdoctoral researcher in Risse's electrochemistry group. Their results also allowed to evaluate the influence of the electrolyte on particle formation. The multimodal measuring cell, which Müller developed together with Risse, contains various sensors: they record the electrochemical impedance, the temperature, but also mechanical forces on the electrodes. In addition, the pouch cell is illuminated with X-rays during the entire discharging/charging cycle (operando) thus creating several radiographies from which the chemical deposition processes can be deduced.

In order to make further progress on the basis of this cell format, a pouch cell laboratory was already set up in 2021. To produce these cells, rectangular electrodes in credit card format are stacked on top of each other and – separated only by a thin separator foil – placed in a sealable pocket (pouch). Compared to coin cells, pouch cells require only a small amount of electrolyte to ensure charge transport. “This has a very strong effect on these processes and must therefore be investigated directly in an industrially relevant cell format,” says Risse. *arö*



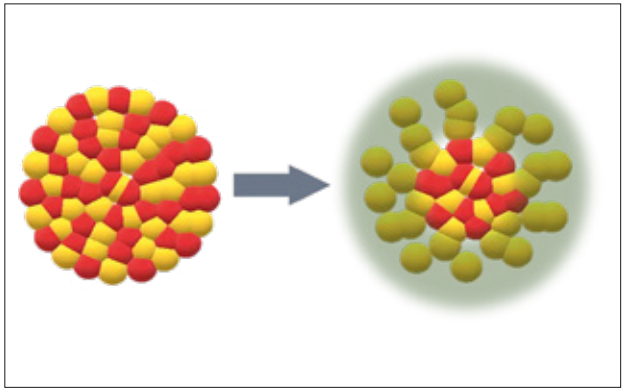
The radiographies of the cell before (left) and after the first discharge (centre) as well as after the first recharge (right). The accumulation of Sulphur-containing particles (bright spots) is visible. This combination of methods allows to compare pouch cells with different electrolytes and additives.

© R. Müller, S. Risse/HZB

Advanced Energy Materials (2022): Operando Radiography and Multimodal Analysis of Lithium-Sulfur Pouch Cells – Electrolyte Dependent Morphology Evolution at the Cathode. R. Müller, I. Manke, A. Hilger, N. Kardjilov, T. Boenke, F. Reuter, S. Dörfler, T. Abendroth, P. Härtel, H. Althues, S. Kaskel, S. Risse. **DOI: 10.1002/aenm.202103432**

NANOSTRUCTURED NICKEL SILICIDE SHINES AS A CATALYST

Electrical energy from wind or sun can be stored as chemical energy in hydrogen. The prerequisite for this, however, is efficient electrolysis of water with inexpensive catalysts. For the production of catalyst materials based on nickel, a corrosion-resistant and hardly toxic metal, energy-intensive high-temperature processes have mostly been used up to now. A team from HZB and TU Berlin led by Prashanth Menezes has found a "soft chemical" way to produce an efficient catalyst. "We combined the element nickel with silicon, the second most abundant element in the Earth's crust, and achieved nanostructuring via a chemical reaction. The resulting material has excellent catalytic properties," says Menezes.



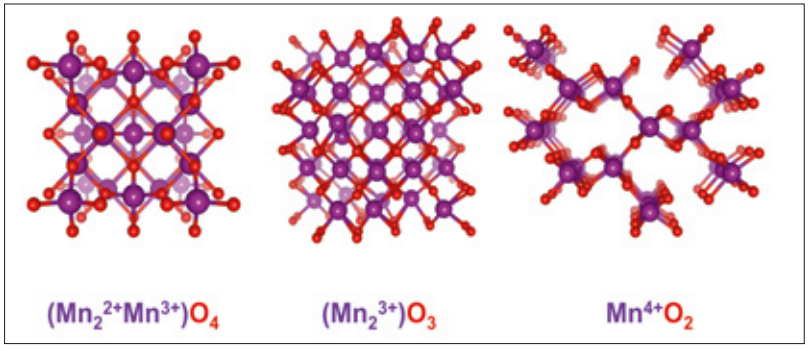
Crystalline nickel silicide (left) is chemically transformed into nanostructured material with excellent catalytic properties for the electrolytic splitting of water and the production of valuable nitrile compounds.

© P. Menezes /HZB/TU Berlin

Compared to modern catalysts based on Nickel, Cobalt, Iron, Ruthenium and Iridium, the nanoporous Ni_2Si is significantly more active and remains stable for longer reaction time at industrial-level conditions. To understand the behavior of Ni_2Si in more detail, the team combined different measurement methods, including elemental analyses, electron microscopy and modern spectroscopic measurements at BESSY II. "In the future, even industrial alkaline water electrolysers could be equipped with a coating of this nanoporous nickel silicide," says Menezes. *arö*

Advanced Energy Materials (2022): Nanostructured Intermetallic Nickel Silicide (Pre)Catalyst for Anodic Oxygen Evolution Reaction and Selective Dehydrogenation of Primary Amines. I. Mondal, J. N. Hausmann, G. Vijaykumar, S. Mebs, H. Dau, M. Driess, and P. W. Menezes. **DOI: 10.1039/D1EE00650A**

GREEN HYDROGEN: FASTER PROGRESS WITH MODERN X-RAY SOURCES



Manganese oxides come in many different structural variants. They are an exciting class of materials for electrocatalysts.

© M. Risch/HZB

Just like nanostructured nickel silicide (see adjacent article), manganese oxides are also considered an exciting class of materials for electrocatalysts for the production of green hydrogen. Marcel Risch and his Young Investigator Group Oxygen Evolution Mechanism Engineering are investigating an important process in the electrocatalysis of water to make it more economically efficient.

Manganese oxides occur in many different structural variants. "A decisive criterion for suitability as an electrocatalyst is the oxidation number of the material and how it changes in the course of the reaction," explains Risch. X-ray absorption spectroscopy (XAS) provides information about this. Risch's team has constructed an electrolysis cell that enables XAS measurements during electrolysis. Combined with electrochemical measurements, the measurement data thus provide a much better understanding of the material during electrocatalysis. The required high intensity of the X-rays is available at the modern synchrotron light source BESSY II. Risch still sees great potential for the application of XAS on the way to inexpensive, environmentally friendly and, above all, long-lasting catalysts.

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Angewandte Chemie (2022): What X-ray absorption spectroscopy can tell us about the active state of earth-abundant electrocatalysts for the oxygen evolution reaction. M. Risch, D. M. Morales, J. Villalobos, D. Antipin. **DDOI: 10.1002/ange.202211949**

PHOTOCATALYSIS: PROCESSES IN CHARGE SEPARATION RECORDED EXPERIMENTALLY

Splitting water into hydrogen and oxygen with the help of photocatalytically active particles could produce green hydrogen cheaply in the future: Sunlight activates charge carriers in photocatalysts, whose spatial separation plays a decisive role in photocatalytic water splitting. However, today's photocatalysts are still either very expensive or not very efficient.

Metal oxide particles are considered favorable candidates with great potential. However, when charge carriers are activated by light, several processes overlap that take place at different speeds and on different spatial scales. To observe such processes experimentally, methods are needed that offer time resolutions down to femtoseconds, but can also observe longer processes that occur within microseconds and slower.

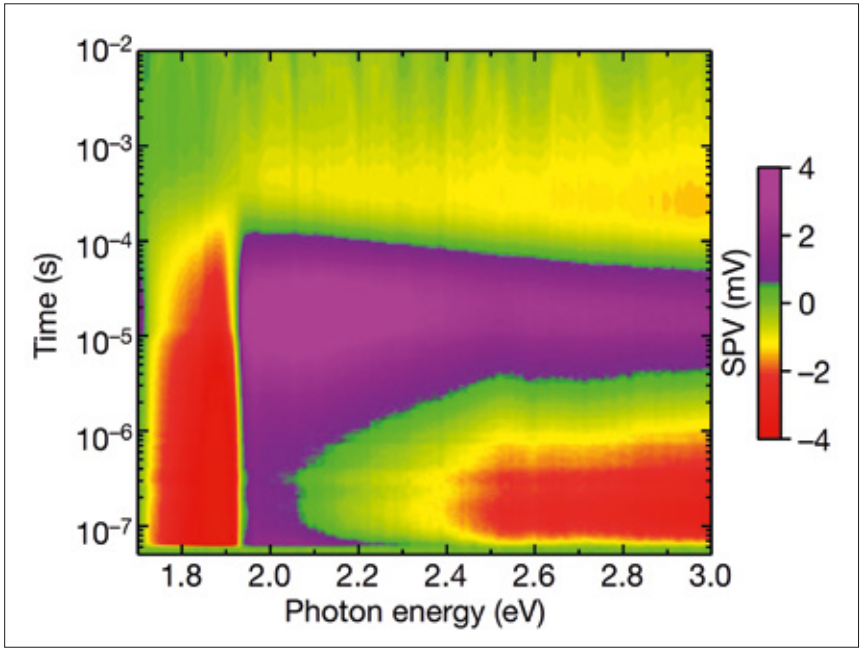
Fast and slow processes

This has now been achieved on microcrystalline copper(I) oxide particles by a team led by Fengtao Fan and Can Li from the Dalian National Laboratory for Clean Energy, China. Using rapid successive time-resolved photoemission electron microscopy images, the scientists showed that one of these processes occurs extremely quickly in Cu_2O particles – in less than picoseconds (10^{-12} s): After excitation with light, electrons are transferred quasi-ballistically to {001} facets of Cu_2O particles.

However, to experimentally observe a second process, a different method was required: because photogenerated "holes" migrate to {111} facets and are trapped there by defects. Thomas Dittrich was able to observe this important process using transient surface photovoltage spectroscopy (SPV spectroscopy), a method he developed at HZB. "We found that hole trapping occurred relatively slowly, over the course of microseconds," he explains.

Versatile method to analyse semiconductors

Taken together, the results make it possible for the first time to study and better understand processes that limit photocatalysis on microcrystalline particles with high spatial and temporal resolution over wide ranges. "With transient SPV spectroscopy, we can also investigate other semiconductors and interfaces that are relevant, for example, for applications ranging from photovoltaics and photocatalysis to high-performance electronics," says Dittrich. Interesting insights into relaxation processes can also be gained from organic semiconductors or ultra-wideband semiconductors such as diamond. "Perhaps our publication in Nature spreads the message how useful this versatile method can be," says Dittrich.



Contour plot of EH-Cu_2O. The photovoltages are plotted as a function of photon energy (x-axis) and time (y-axis). Positive SPV signals (purple regions above 1.9 eV) correspond to the relaxation of holes trapped on {111} facets, whereas negative SPV signals (red regions) correspond to the relaxation of electrons trapped on {001} facets. © T. Dittrich/HZB

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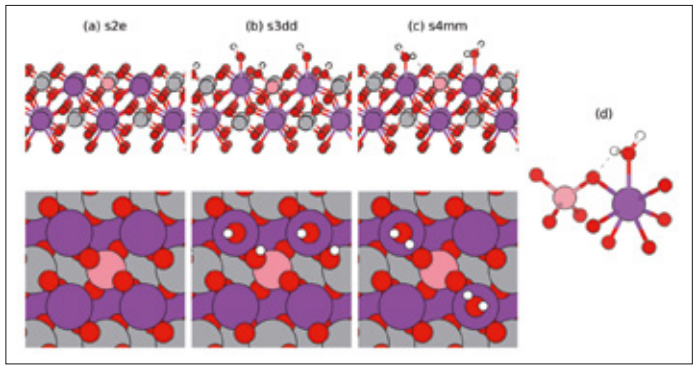
Nature (2022): Spatiotemporal imaging of charge transfer in photocatalyst particles. R. Chen, Z. Ren, Y. Liang, G. Zhang, T. Dittrich, R. Liu, Y. Liu, Y. Zhao, S. Pang, H. An, C. Ni, P. Zhou, K. Han, F. Fan and C. Li. **DOI: 10.1038/s41586-022-05183-1**

HOW PHOTOELECTRODES CHANGE IN CONTACT WITH WATER



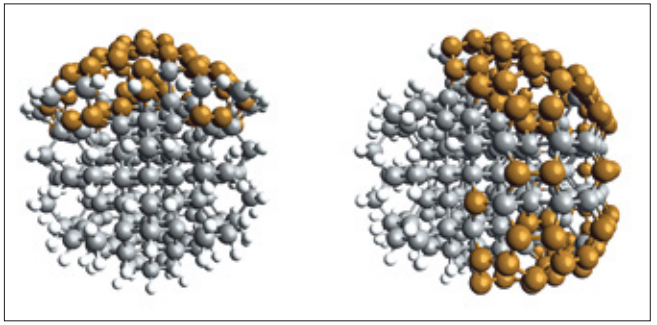
Investigation of the formation of polarons at $BiVO_4$: (a) pristine surface slab with surface polaron, (b) single-hydroxylated surface polaron with dissociated water molecules, and (c) surface polaron with two water molecules oriented toward a particular VO_4. Bi atoms are shown in purple, V atoms in gray, O atoms in red, and H atoms in white; the pink V atom denotes the site at which an electron polaron is initialized to form. The local coordination environment of Bi and V of the main structural moiety in this study is shown in (d). © W. Wang et al.

Photoelectrodes based on $BiVO_4$ are considered top candidates for an inexpensive and efficient solar hydrogen production. Until now, however, it was not clear what effects contact with water molecules has on the electronic properties of the surface. David Starr and Marco Favaro from the HZB Institute for Solar Fuels have investigated this question. They studied single crystals of $BiVO_4$ doped with molybdenum under water vapor with resonant ambient pressure photoemission spectroscopy at the Advanced Light Source at Lawrence Berkeley National Laboratory.

A team led by Giulia Galli at the University of Chicago then performed density functional theory calculations to help interpret the data and to untangle the contributions of individual elements and electron orbitals to the electronic states. The combination of measurements and calculations showed that due to excess charge, generated by either doping or defects on certain surfaces of the crystal, so-called polarons may form: negatively charged localized states, where water molecules can easily attach and then dissociate. The results provide valuable insights and might foster the design of better photoanodes for green hydrogen production. *arö*

J Am Chem Soc. (2022): Influence of Excess Charge on Water Adsorption on the $BiVO_4(0_{10})$ Surface. W. Wang, M. Favaro, E. Chen, L. Trotochaud, H. Bluhm, K.-S. Choi, R. van de Krol, D. E Starr, G. Galli. **DOI: 10.1021/jacs.2c07501**

NANODIAMONDS CAN BE ACTIVATED AS PHOTOCATALYSTS WITH SUNLIGHT



The illustration shows two variants of nanodiamond materials with different surfaces: $C_{230}H_{106}$ on the left, $C_{286}H_{68}$ on the right. Sp^3 C atoms (diamond) black, sp^{3-x} C atoms (fullerene-like) brown, H atoms: Light grey. © T. Kirschbaum/HZB

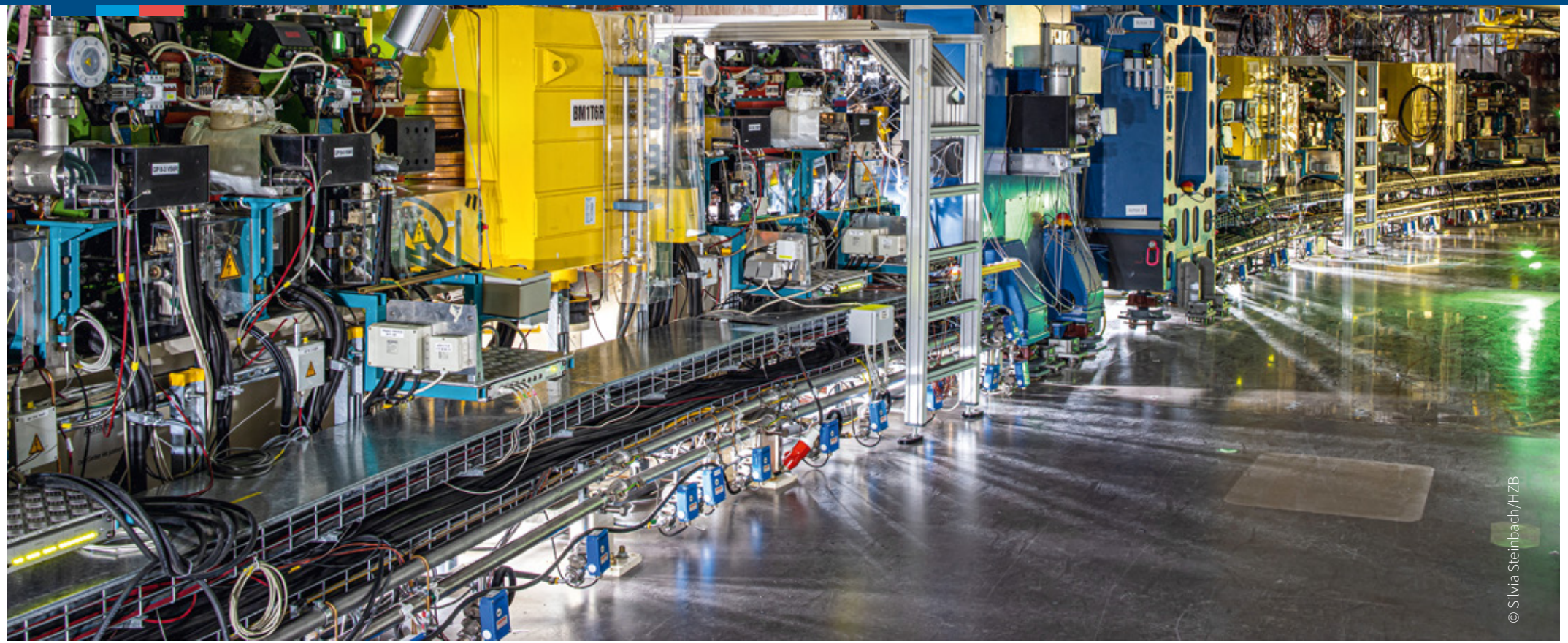
In order to catalytically accelerate chemical reactions in an aqueous medium, electrons from the catalyst need to go into solvation. This can be achieved with light. So-called nanodiamond materials have therefore been the focus of research for some years: they are inexpensive nanoparticles made of carbon whose surfaces are very large compared to their volume. However, they require high-energy UV light for excitation. Because they are so extremely tiny, new molecular states can establish themselves on the surfaces under certain circumstances that also absorb visible light.

A team at HZB has investigated different variants of nanodiamond materials during excitation with UV and visible light. The processes were analyzed with extremely high time resolution. “The hydrogen on the surfaces makes electron emission much easier,” explains Tristan Petit, nanodiamond expert at HZB. “A certain combination of hydrogen as well as fullerene-like carbon on the surfaces of the nanoparticles is ideal,” he says. The theory team led by Annika Bande contributed modelling with density functional theory to interpret the spectra. The work shows that the emission of solvated electrons from nanodiamonds in water is possible with visible light and that nanodiamond materials are suitable as photocatalysts. *arö*

Nanoscale (2022): Early dynamics of the emission of solvated electrons from nanodiamonds in water. F. Buchner, T. Kirschbaum, A. Venerosy, H. Girard, J.-C. Arnault, B. Kiendl, A. Krueger, K. Larsson, A. Bande, T. Petit, C. Merschjann. **DOI: 10.1039/D2NR03919B**

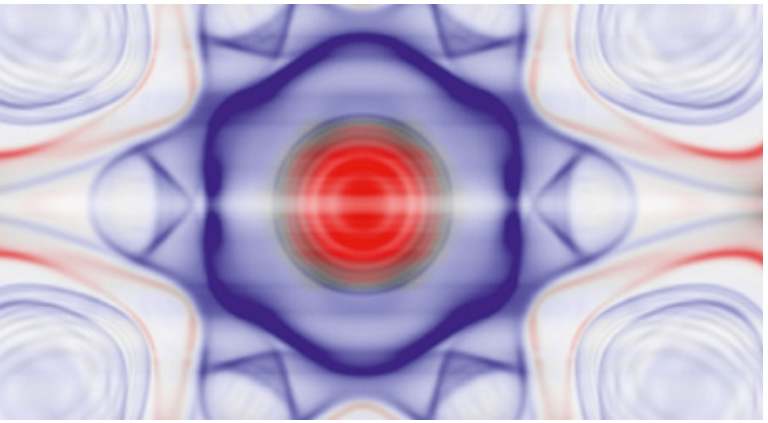
HIGHLIGHTS FROM OUR RESEARCH – INFORMATION

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, the access speed to stored content as well as the energy consumption of information technology and to open up new areas of application. **There is a scientific publication for almost every article. Click on this symbol for it:**



BUCKYBALLS ON GOLD ARE LESS EXOTIC THAN GRAPHENE

Graphene consists of carbon atoms that crosslink in a plane to form a flat honeycomb structure. In addition to surprisingly high mechanical stability, the material has exciting electronic properties: The electrons behave like massless particles, which can be clearly demonstrated in spectrometric experiments. A recent study suggested that it is infinitely easier to make artificial graphene using C_{60} molecules called buckyballs. Only a uniform layer of these needs to be vapor-deposited onto gold for the gold electrons to take on the special graphene properties.



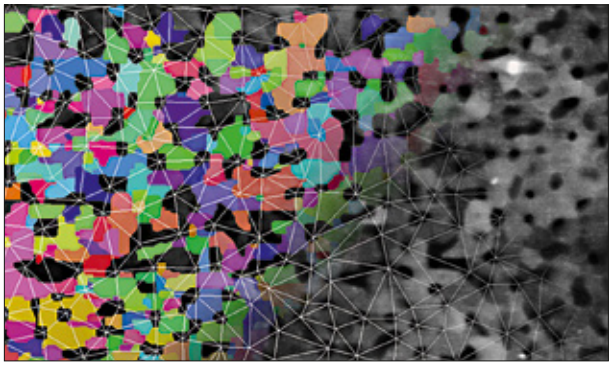
Using density functional theory and measurement data from spin-resolved photoemission, the team investigated the origin of the repeating Au(111) bands and resolved them as deep surface resonances. These resonances lead to an onion-like Fermi surface of Au(111) . ©HZB

A team led by Andrei Varykhalov has teted this effect experimentally. They used angle-resolved ARPES spectroscopy at BESSY II, which enables particularly precise measurements, and also analysed electron spin for some measurements. "We see a parabolic relationship between momentum and energy in our measured data, so it's a very normal behavior," explains Maxim Krivenkov, lead author of the study. "These signals come from the electrons deep in the gold or copper substrate and not the layer, which could be affected by the buckyballs." Therefore, the buckyball layer on gold cannot be considered an artificial graphene. *arö*

Nanoscale (2022): On the problem of Dirac cones in fullerenes on gold. M. Krivenkov, D. Marchenko, M. Sajedi, A. Fedorov, O. J. Clark, J. Sánchez-Barriga, E. D. L. Rienks, O. Rader, and A. Varykhalov. **DOI: 10.1039/D1NR07981F**

THERMAL INSULATION FOR QUANTUM TECHNOLOGIES

New energy-efficient IT components often only operate stably at extremely low temperatures. Therefore, very good thermal insulation of such elements is crucial. A team led by Klaus Habicht from HZB has now taken a big step forward in this direction. Using a novel sintering process, they produced samples of silicon and silicon aluminum to which microstructures that suppress heat transport were added by means of electrochemical etching.



Electron microscope image of a silicon sample with nanocrystallites of different orientation (coloured), pores (black) and the pore network recognised by the image processing software (white grid lines). ©: D. Kojda/HZB

Heat conduction works via vibrations of the crystal lattice, so called phonons. However, these phonons can only propagate if they do not encounter obstacles on which they are scattered. Pores as well as nanoparticles and domain boundaries with suitable distances and diameters can become such scattering centers and thus reduce heat conduction. Using a model, the scientists calculated the behavior of the phonons and thus the thermal conductivity in samples with different microstructures. "With this model, we can clearly separate the contributions of nanoparticles and pores to thermal conductivity," Habicht explains. The experimental results obtained at the HZB's scanning electron microscope confirm the new model. "Understanding the basic transport processes helps us to produce and further develop customized materials with strongly reduced thermal conductivity in a targeted manner," says Danny Kojda, the first author of the study. *arö*

Nano Research (2022): Characterization and modeling of the temperature-dependent thermal conductivity in sintered porous silicon-aluminum nanomaterials. D. Kojda, T. Hofmann, N. Gostkowska-Lekner, and K. Habicht. **DOI: 10.1007/s12274-022-4123-y**

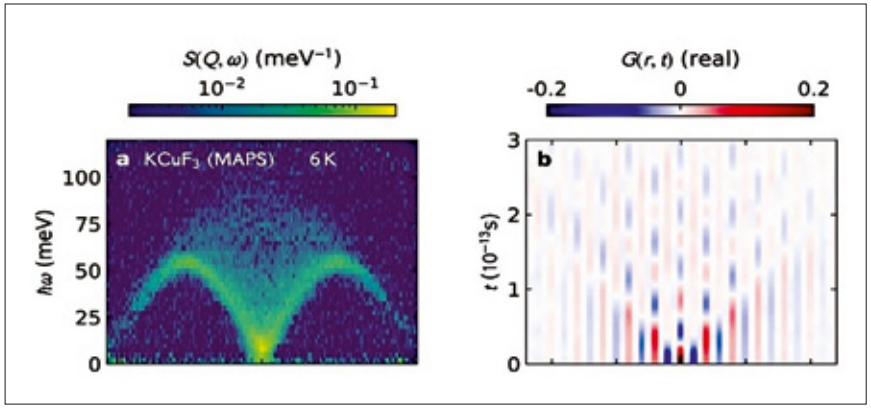
QUANTUM MATERIALS: DYNAMICS IN ONE-DIMENSIONAL SPIN CHAINS NEWLY ELUCIDATED

Quantum materials are characterized by macroscopic properties that are mainly shaped by the quantum physical wave function of electrons. They can be attributed in part to interactions between electrons, as in ferromagnetism, antiferromagnetism and superconductivity. However, there are also phenomena that depend on the topological character of the wave function, for example in topological insulators and Dirac semimetals. Potential applications of quantum materials include spin-based electronics (spintronics) and quantum computers.

Neutron scattering is considered the method of choice for investigating magnetic structures and excitations in quantum materials. The evaluation of measurement data from the 2000s with new methods has provided much deeper insights into a model system – the 1D Heisenberg spin chains. A new toolbox is available for elucidating future quantum materials has been achieved. Potassium copper fluoride $KCuF_3$ is considered the simplest model material realising the so-called Heisenberg quantum spin chain: The spins interact with their neighbors antiferromagnetically along a single direction (one-dimensional), governed by the laws of quantum physics.

Dynamics like a wake

"We carried out the measurements on this simple model material at the ISIS spallation neutron source some time ago when I was a postdoc," says Bella Lake, who heads the HZB-Institute Quantum Phenomena in Novel Materials and is a member of the Topic "Quantum Materials" in Program 2 of the Helmholtz Research Field Information. "We published our results in 2005, 2013 and again in 2021 comparing to new theories each time they became available," she says. Now with new and extended methods, a team led by Alan Tennant and Allen Scheie have succeeded to gain significantly deeper insights into the interactions between the spins and their spatial and temporal evolution.



The data from neutron scattering (left) provide information about absorbed energies in reciprocal space. With the new evaluation, it has been possible to obtain statements about new magnetic states and their temporal development in real space (right). The colours blue and red indicate the two opposite spin directions. © HZB

"With neutron scattering, you sort of nudge a spin so that it flips. This creates a dynamic, like a wake when a ship is sailing through water, which can affect its neighbors and their neighbors," Tennant explains.

New tool box

"Neutron scattering data is measured as a function of energy and wavevector," says Scheie. "Our breakthrough was to map the spatial and temporal development of the spins using mathematical methods such as a back-Fourier transformation." Combined with other theoretical methods, the team obtained information about interactions between the spin states and their duration and range, as well as insights into the so-called quantum coherence, which is considered to be the cause of certain macroscopic properties.

The work demonstrates a new tool box for the analysis of neutron scattering data and might foster a deeper understanding of quantum materials that are relevant for technological use.

red.

Nature Communications (2022): Quantum wake dynamics in Heisenberg antiferromagnetic chains. A. Scheie, P. Laurell, B. Lake, S. E. Nagler, M. B. Stone, J.-S. Caux, and D. A. Tennant. **DOI: 10.1038/s41467-022- 33571-8**

HOW ELECTRON SPIN COUPLING AFFECTS CATALYTIC OXYGEN ACTIVATION

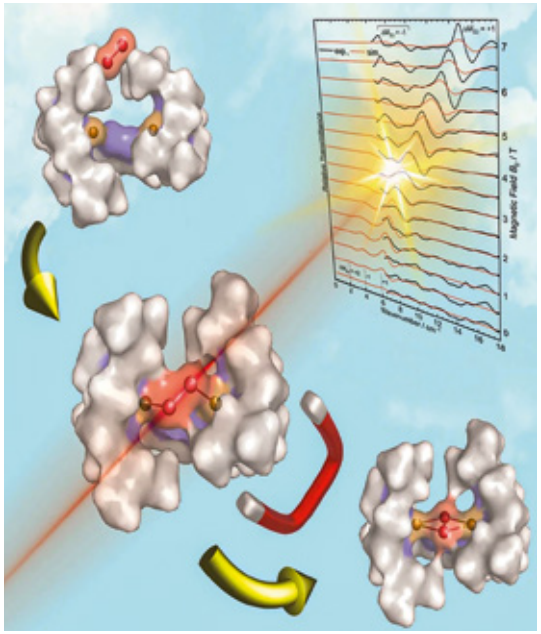


Illustration: catalytic activation of molecular oxygen by copper complexes. © T. Lohmiller/HZB

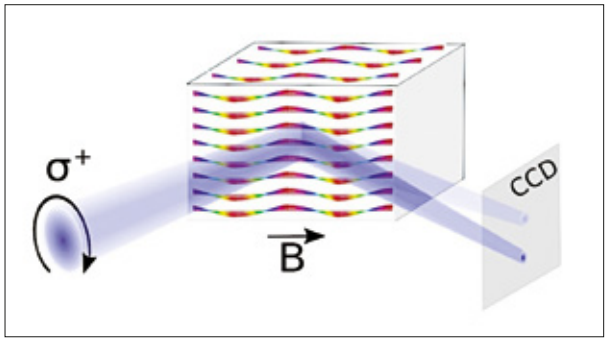
Molecular oxygen (O_2) is a preferred oxidant in green chemistry. However, activation of O_2 and control of its reactivity requires precise adjustment of the spin states in the reactive intermediates. In nature, this is achieved by metalloenzymes that bind O_2 at iron or copper ions. In the case of type III dicopper metalloproteins involved in oxygen transport and oxygenation of phenolic substrates, little was known about the precise process. Through a sophisticated ligand design, a research group of the University of Göttingen has succeeded in isolating a series of model complexes that mimic the initial stage of oxygen binding at dicopper sites.

A team at the EPR4Energy joint lab of HZB and Max Planck Institute for Chemical Energy Conversion complemented this breakthrough in chemical synthesis with a new approach of THz-EPR spectroscopy. The new method allowed to investigate the function-determining antisymmetric exchange in coupled dicopper(II) complexes and to detect the entirety of spin state transitions in the system. “In addition to the knowledge gained about this important system, our method opens up the possibility of studying previously inaccessible spin-spin interactions in a variety of novel catalytic and magnetic materials,” explains Thomas Lohmiller, one of the first authors of the study. *arö*

JACS Au (2022): Antisymmetric Spin Exchange in a μ-1,2-Peroxodicopper(II) Complex with an Orthogonal Cu–O–O–Cu Arrangement and S = 1 Spin Ground State Characterized by THz-EPR. T. Lohmiller, C. Spyra, S. Dechert, S. Demeshko, E. Bill, A. Schnegg, and F. Meyer. **DOI: 10.1021/jacsau.2c00139**

SPINTRONICS: A NEW TOOL AT BESSY II FOR CHIRALITY INVESTIGATIONS

Information on complex magnetic structures is crucial to understand and develop spintronic materials. With ALICE II, a new instrument is available at BESSY II to obtain precisely this information. It was developed as part of a project funded by the German Federal Ministry of Education and Research and HZB by Florin Radu and the technical design department at HZB in close cooperation with Christian Back from the Technical University Munich. “ALICE II has a unique capability, namely to allow for magnetic X-ray scattering in reciprocal space using a new large area detector, and this at up to the highest allowed reflected angles,” Radu explains.



The picture reflects the main effect: A circular polarized soft-X-ray beam scatters off a crystal that exhibits a helical or conical magnetic order. This leads to two scattered beams of different intensity. © F. Radu/HZB

To demonstrate the performance of the new instrument, the scientists examined a polished sample of Cu_2OSeO_3. This is a Mott insulator with a cubic crystal structure which lacks inversion symmetry. The group could observe helical and conical magnetic modulations as satellite reflections around the specular peak via x-ray magnetic scattering with circularly polarized x-rays. “What‘s more: the chirality information of the underlying spin textures is encoded as its dichroic intensity,” Radu points out. These results pave a novel way to investigate chiral and polar magnetic textures with ultimate spatial resolution and at the very short time scales typical to synchrotron X-ray experiments. *arö*

Science and Technology of Advanced Materials (2022): Chiral surface spin textures in Cu_2OSeO_3 unveiled by soft x-ray scattering in specular reflection geometry. V. Ukleev, C. Luo, R. Abrudan, A. Aqeel, C. H. Back, and F. Radu. **DOI: 10.1080/14686996.2022.2131466**

A NEW ROAD TOWARDS SPIN-POLARIZED CURRENTS

The second half of the 20th century was the age of electronics. Electronic devices became miniaturized and even more complex, creating problems for their energy consumption and waste heat. Spintronics promises to store or transport information based on spins alone, which would work faster with much less energy. Unfortunately, it is still a challenge to control spin in a material by external fields reliably and at scale.

The transition metal dichalcogenide (TMD) series are the most intensely studied quasi two-dimensional materials beyond graphene, with charge density waves, superconductivity and non-trivial topological all commonplace across the material family. Hafnium diselenide ($HfSe_2$) belongs to this class of materials.

From electronics to spintronics

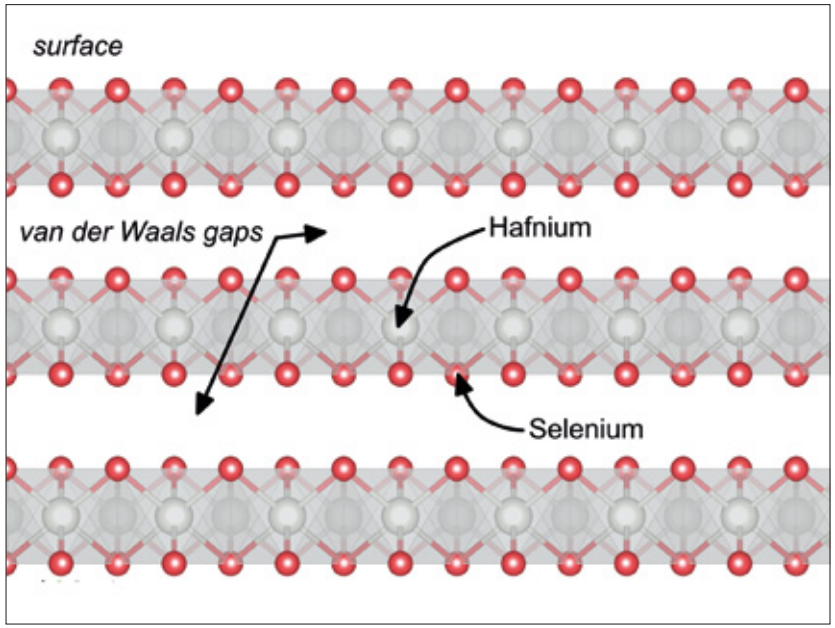
A team of scientists at BESSY II has unveiled a new property of the electronic structure of $HfSe_2$ that could lead to a more convenient route to generate and control spin currents. “In order to shift from electronics to spintronics, we have to find materials wherein spin up and spin down electrons behave differently,” first author Oliver Clark explains. There are two ways to do this, he points out: “We can either externally perturb the material so that electrons of different spins become functionally inequivalent, or we can use magnets where the electrons of opposite spins are functionally different intrinsically.”

For the first method, the difficulty lies in finding suitable pairings of materials and mechanisms by which spin control can be externally imposed. For example, in the so-called 2H structured transition metal dichalcogenides, one needs perfect single crystals and a circularly polarized light source. By contrast, the second method is much easier, but integrating magnets into devices is problematic for the operation of conventional electronic components, especially on small scales.

Linearly polarized light does do the trick

Between those two ways, a middle ground exists, at least for some select materials such as $HfSe_2$. “If you probe this material with linearly-polarized light – which is easier to produce than circularly polarized light – the material acts as a magnet in terms of its spin-structure,” explains Clark. “So the spin-selectivity becomes very easy, but you do not have the problems associated with other magnetic properties.” The advantage: Crystal quality or orientation of the sample no longer matter.

This provides an entirely new route towards the generation of spin-polarized currents from transition metal dichalcogenides. The physicists are very excited about the implications of this work. “Our results are of relevance not only to physicists concerned with layered two-dimensional materials, but as well to specialists in spintronic and opto-spintronic device fabrication,” Clark says. *arö*

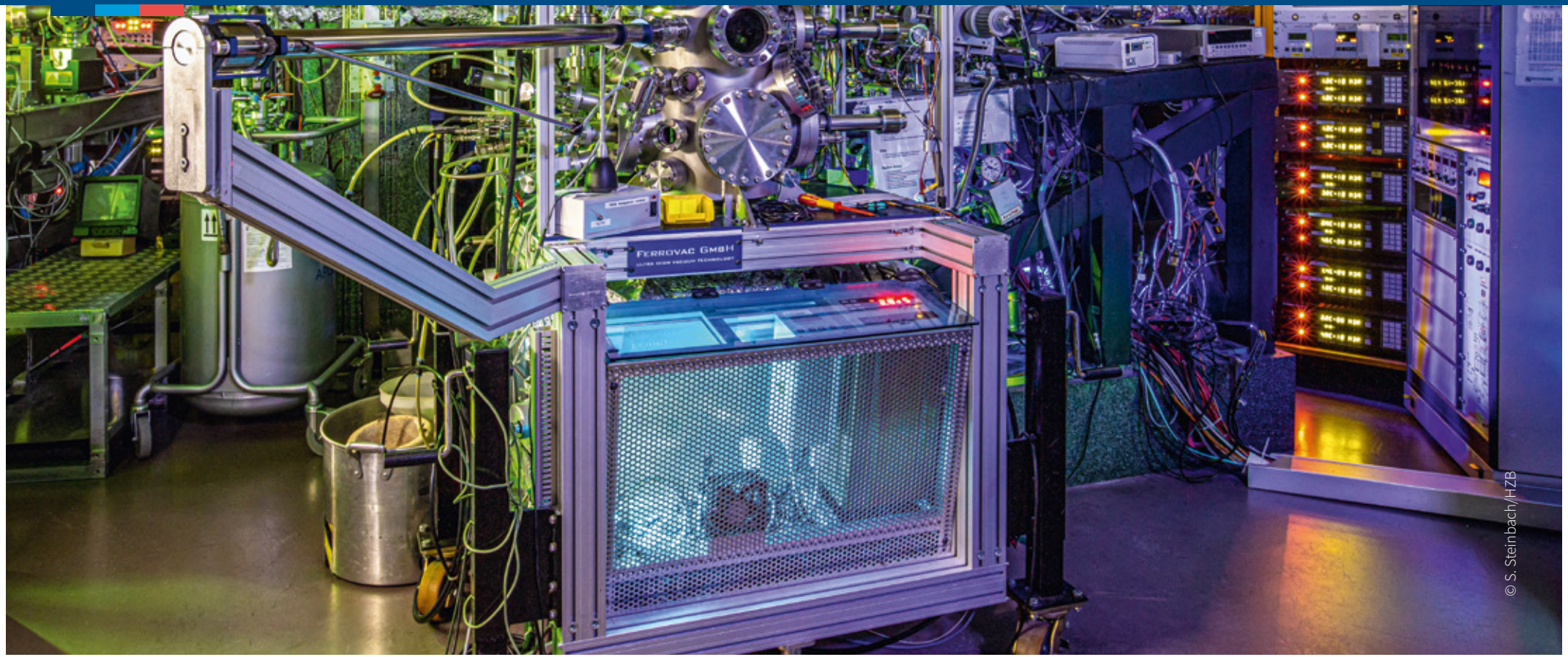


Hafniumdiselenide is a quasi-two-dimensional material with interesting properties for spintronics. Here, its crystal structure is shown. O.Clark/HZB

Nature Communications (2022): AHidden spin-orbital texture at the Γ-located valence band maximum of a transition metal dichalcogenide semiconductor. O. J. Clark, O. Dowinton, M. S. Bahramy and J. Sánchez-Barriga. **DOI: 10.1038/s41467-022-31539-2**

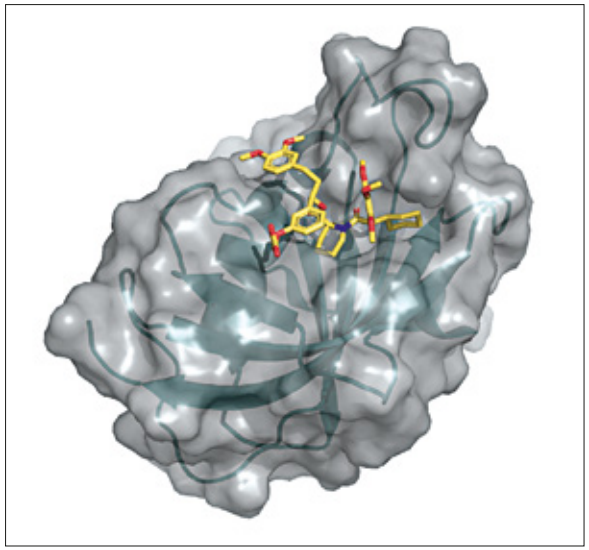
HIGHLIGHTS FROM OUR RESEARCH – MATTER

To enable deep insights into matter, the X-ray source BESSY II and its instruments are constantly being further developed. The versatile measuring instruments and powerful operation of BESSY II enable first-class materials research at HZB and attract numerous domestic and international research guests to Berlin – Work by guest researchers at BESSY II can be recognized by this symbol N. **There is a scientific publication for almost every article. Click on this symbol for it:**



4000TH PROTEIN STRUCTURE DECODED AT BESSY II

The MX beamlines at the X-ray source BESSY II specialise in the highly automated structural analysis of protein crystals. They enable a high throughput of samples, which is why the 4,000th protein structure could already be decoded in 2022. The demand for measurement times comes both from basic research and from user groups in industry.



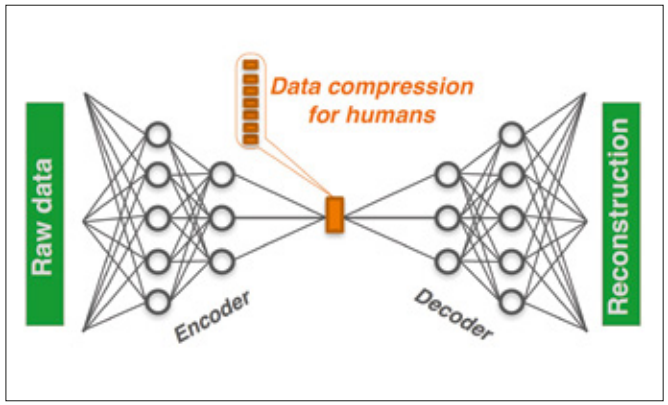
3D structure of the protein FKBP51, which was studied as the 4,000th protein structure at BESSY II. © J. A. Lerma Romero

For the 4,000th protein structure studied, the team led by Felix Hausch from the Techcal University of Darmstadt had produced crystals from the protein molecule FKBP51 and examined them on the MX beamlines. FKBP51 plays a special role in major health problems of our time. It regulates the signal transduction of steroid hormone receptors. Stress can disrupt this transmission, which can lead to depression, chronic pain or diseases such as diabetes and obesity. The protein FKBP51 is considered a promising target for drugs against these diseases. “The protein structure analysis shows us where interesting “pockets” are located in the molecule that could be possible drug targets,” says Christian Meyners from the TU Darmstadt team. The result is stored in the Protein Data Bank, which contains all experimentally determined protein structures. *arö*

Front. Mol. Biosci. (2022): Binding pocket stabilization by high-throughput screening of yeast display libraries. J. A. Lerma Romero, C. Meyners, A. Christmann, L. M. Reinbold, A. Charalampidou, F. Hausch, H. Kolmar. **DOI: 10.3389/ fmolb.2022.1023131**

NEW SOFTWARE BASED ON AI HELPS TO INTERPRET COMPLEX DATA

Experimental data is often not only highly dimensional, but also noisy and full of artefacts. This makes it difficult to interpret the data. Now, new software developed at HZB based on artificial intelligence methods can help: It is a special class of neural networks (NN) that experts call “disentangled variational autoencoder network (β-VAE)”. Put simply, the first NN takes care of compressing the data, while the second NN subsequently reconstructs the data. “In the process, the two NNs are trained so that the compressed form can be interpreted by humans,” explains Gregor Hartmann. The physicist and data scientist supervises the Joint Lab on Artificial Intelligence Methods at HZB, which is run by HZB together with the University of Kassel.



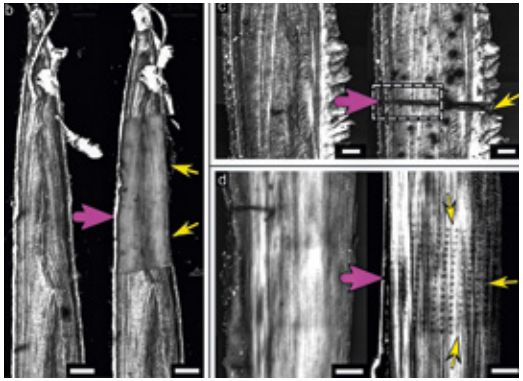
With the help of special neural networks, raw data can first be compressed and then reconstructed in such a way that it can be interpreted by scientists. © G. Hartmann et al.

This enables to recognize correlations that would otherwise not be discernible. The team led by Hartmann used the software to determine the photon energy of the FLASH free electron laser at DESY from single photoelectron spectra. On the other hand it is suitable for very different applications in science and is really good when it comes to impaired data. “We hope that soon many colleagues will come with their data and we can support them,” Hartmann says.

arö

Scientific Reports (2022): Unsupervised realworld knowledge extraction via disentangled variational autoencoders for photon diagnostics. G. Hartmann, G. Goetzke, S. Düsterer, P. Feuer-Forson, F. Lever, D. Meier, F. Möller, L. Vera Ramirez, M. Guehr, K. Tiedtke, J. Viefhaus, and M. Braune. **DOI: 10.1038/s41598-022-25249-4**

HIGH-ENERGY X-RAYS LEAVE A TRACE OF DESTRUCTION IN BONE COLLAGEN



The images (b) show the collagen distribution in pike bones before (left) and after (right) a µCT experiment and (c) before (left) and after (right) an X-ray diffraction µCT experiment at the mySpot beamline, BESSY. Also (d) before (left) and after (right) a 2D mapping XRD mySpot experiment. The damaged areas appear dark marked with yellow arrows. Arrows in pink show the x-rays. © Charité Berlin/HZB

Beyond a certain dose, X-rays damage living tissue, so there are clear medical indications for X-rays to keep radiation exposure to an unavoidable minimum. In basic research, the opposite has been true until now. “More flux and higher energy is better, because you can achieve greater depth of field and higher resolution with more intense X-rays,” says Paul Zaslansky from Charité-Universitätsmedizin. Zaslansky and his team have now analyzed bone samples from fish and mammals at the MySpot beamline at BESSY II.

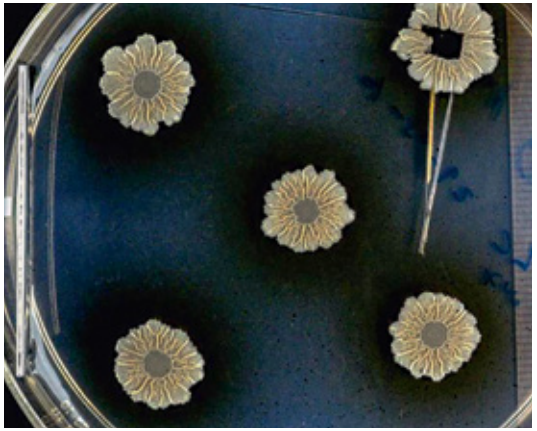
BESSY II generates a well characterized broad-range of X-rays, precisely focused in an intermediate energy range which allows insights into the finest structures and even chemical and physical processes in materials. “Thanks to sensitive detectors and rather mild irradiation conditions in BESSY II we were able to demonstrate on our various bone samples that collagen fibres become damaged by the irradiation absorption in the mineral nanocrystals,” Zaslansky summarises the results of the study. “The high-energy photons from the X-ray light trigger a cascade of electron excitations. Ionisaton of calcium and phosphorus in the mineral then damages proteins like collagen in bone,” first author Katrein Sauer says. So, as everywhere in medicine, it comes down to using a minimal dose to get the insights that reflect the material condition without causing damage.

arö

Nature communications (2022): Primary radiation damage in bone evolves via collagen destruction by photoelectrons and secondary emission self-absorption. K. Sauer, I. Zizak, J.-B. Forien, A. Rack, E. Scoppola, and P. Zaslansky. **DOI: 10.1038/s41467-022-34247-z**

WHAT HAPPENS IN BIOFILMS?

Most bacteria have the ability to form communities, biofilms, that adhere to a wide variety of surfaces and are difficult to remove. This can lead to major problems, for example in hospitals or in the food industry. An international team of researchers led by Hebrew University, Jerusalem, and the B CUBE at the TU Dresden, has investigated a model system for biofilms from the bacterium *Bacillus subtilis*, which is useful for plants, among others at BESSY II.



When bacteria join together to form communities, they may build complex structures. The photo shows wild-type *Bacillus subtilis* biofilms.

© L. Chai/HUJI

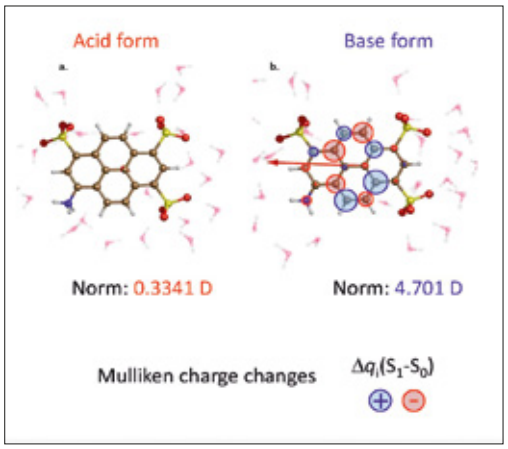
At the MySpot beamline of BESSY II, the scientists were able to spatially resolve the structures within the biofilm and distinguish well between matrix components, bacterial cells, spores, and water. “X-ray fluorescence spectroscopy is a method that allowed us to identify important metal ions such as calcium, zinc, manganese, and iron, even when present in trace amounts,” says Ivo Zizak, HZB physicist in charge of the MySpot beamline. This made it possible to correlate biofilm morphology and metal ion distribution. The results show that the structures in the matrix not only play an important role in the distribution of nutrients and water, but also actively influence the bacteria's ability to behave as a multicellular organism. “This could help us to better deal with biofilms overall, with the beneficial ones as well as the harmful ones,” says Liraz Chai from the Hebrew University.

arö

PNAS (2022): Multiscale X-ray study of *Bacillus subtilis* biofilms reveals interlinked structural hierarchy and elemental heterogeneity. D. N. Azulay, O. Spaeker, M. Ghrayeb, M. Wilsch-Bräuninger, E. Scoppola, M. Burghammer, I. Zizak, L. Bertinetti, Y. Politi, and L. Chai. **DOI: 10.1073/pnas.2118107119**

AN ULTRAFAST X-RAY GLANCE INTO PHOTOACID ELECTRONIC STRUCTURE

Photoacids are molecules that release a proton upon electronic excitation, thus enhancing the acidity of a liquid. Pioneering work by the German physical chemist Theodor Förster has shown the direct relationship between the wavelength position of optical absorption and acidity properties with which the increase in acidity in the first electronic excited state can be quantified. With the help of ultrafast X-ray spectroscopy, an international team of researchers has been able to clarify the long-standing question of the cause of photoacidity.



Estimated charge distribution changes on the APTS photoacid and conjugate photobase forms, showing major changes in Mulliken charges and in the electric dipole moment upon electronic excitation. © MBI

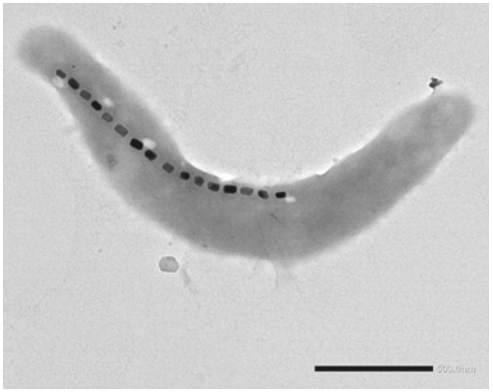
The team investigated the electronic charge distributions of photoacids along their four stages at BESSY II. That provided direct microscopic insight into the electronic structural changes of the proton donating amine group of an aminopyrene derivative in aqueous solution. Together with quantum chemical calculations, such results provide a consistent picture of photoacid behavior: electronic charge distributions of the proton donating group are only minor on the photoacid side, but substantial on the conjugate photobase side. Yet the overall dipole moment change of the whole molecule is as important as the local charge distribution changes. Hence solvation dynamics by the solvent water is the second important factor governing photoacidity.

MBI

Angew. Chem. Int. Ed. (2022): Electronic Structure Changes of an Aromatic Amine Photoacid along the Förster Cycle. S. Eckert, M.-O. Winghart, C. Kleine, A. Banerjee, M. Ekimova, J. Ludwig, J. Harich, M. Fondell, R. Mitzner, E. Pines, N. Huse, P. Wernet, M. Odelius, and E. T. J. Nibbering. **DOI: 10.1002/anie.202200709**

MAGNETIC NANOPARTICLES IN BIOLOGICAL VEHICLES INDIVIDUALLY CHARACTERIZED FOR THE FIRST TIME

Magnetic nanoparticles are promising tools for medical applications. Incorporated into biological vehicles, they can then be steered by external magnetic fields to their place of use in the body, where they can release drugs or destroy cancer cells. However, this requires precise knowledge of the magnetic properties of these nanoparticles. Until now, such information could only be obtained on average over thousands of nanoparticles. Now, a team at HZB has developed a method to determine the characteristic parameters of each individual magnetic nanoparticle.



Under the transmission electron microscope, the bacterial cell is visible in which several magnetic nanoparticles have arranged themselves into a chain. The scale shows 500 nanometres. © L. Marcano/HZB

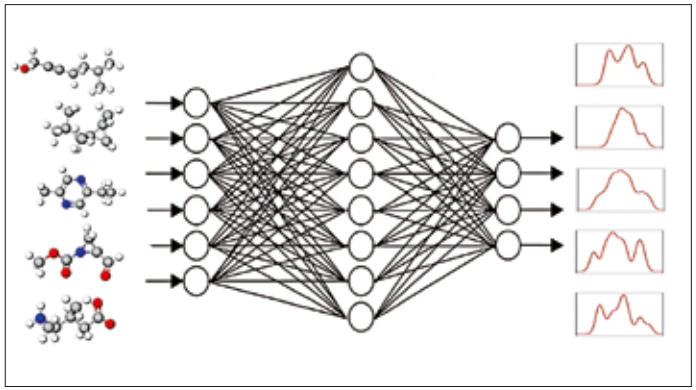
To do this, the researchers combined images taken with the scanning transmission X-ray microscope MAXYMUS at BESSY II with theoretical simulations. This made it possible to precisely determine the magnetic anisotropy of nanoparticles inside a bacterium. The magnetic anisotropy is an important parameter for controlling and steering magnetic nanoparticles as it describes how a magnetic nanoparticle reacts to external magnetic fields applied at an arbitrary direction. Actually, such images can only be made at large scale research facilities, like BESSY II, providing sufficiently intense X-ray radiation. “In the future, however, with the development of compact plasma X-ray sources, this method could become a standard laboratory technique,” says Sergio Valencia.

arö

ACS Nano (2022): Magnetic Anisotropy of Individual Nanomagnets Embedded in Biological Systems Determined by Axi-asymmetric X-ray Transmission Microscopy. L. Marcano, I. Orue, D. Gandia, L. Gandarias, M. Weigand, R. M. Abrudan, A. García-Prieto, A. García-Arribas, A. Muela, M. Luisa Fdez-Gubieda, and S. Valencia. **DOI: 10.1021/acsnano.1c09559**

CALCULATING THE "FINGERPRINTS" OF MOLECULES WITH AI

Biomolecules, large inorganic molecules, but also quantum dots, which often consist of thousands of atoms, can hardly be calculated in advance using conventional methods. But this is a prerequisite for correctly interpreting experimentally obtained data. Annika Bande, a theoretical chemist at HZB, and her team have systematically investigated how computing time can be shortened by using methods from artificial intelligence. To do this, a computer programme from the group of "graphical neural networks" or GNN receives small molecules as input with the task of determining their spectral responses.



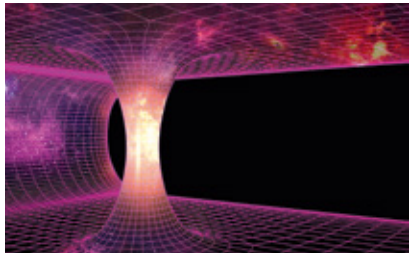
The graphical neural network GNN receives small molecules as input with the task of determining their spectral responses. By matching them with the known spectra, the GNN programme learns to calculate spectra reliably.
© K. Singh, A. Bande/HZB

In the next step, the GNN programme compares the calculated spectra with the known target spectra (DFT or experimental) and corrects the calculation path accordingly. Round after round, the result becomes better. The GNN programme thus learns on its own how to calculate spectra reliably with the help of known spectra. "The accuracy increases by 20 percent and this is done in a fraction of the computation time," says first author Kanishka Singh. "Recently developed GNN frameworks could do even better," Bande says. "And the demand is very high. We therefore want to strengthen this line of research." *arö*

J. Chem. Theory Comput. (2022): **Graph Neural Networks for Learning Molecular Excitation Spectra.** K. Singh, J. Münchmeyer, L. Weber, U. Leser and A. Bande. **DOI: 10.1021/acs.jctc.2c00255**

HOW QUANTUM COMPLEXITY IS GROWING

There is a huge gap between quantum physics and the theory of gravity. Only those who bridge it can describe the behavior of complex quantum many-body systems, for example that of black holes and wormholes in the universe. Now an international group of theorists has proved a mathematical conjecture about the behavior of complexity in such systems, and thus constructed such a bridge. According to this, quantum complexity grows linearly for exponentially long times until it saturates at a point in time that is exponential to the system size. *arö*

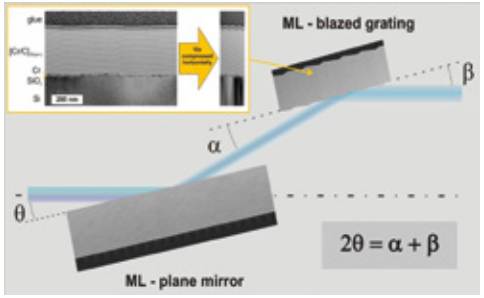


Black holes and wormholes in the universe are complex many body systems and require a deeper understanding of space, time, gravity and quantum physics. ©Trahko/stock.adobe.com

Nature Physics (2022): **Linear growth of quantum circuit complexity.** J. Haferkamp, P. Faist, N. B. T. Kothakonda, J. Eisert and N. Yunger Halpern. **DOI: 10.1038/s41567-022-01539-6**

NEW MONOCHROMATOR OPTICS FOR TENDER X-RAYS

Measurements with high sensitivity and high spatial resolution using X-ray light in the tender energy range of 1.5 to 5.0 keV are ideal for investigating energy materials such as batteries or catalysts, but also biological systems. A team from HZB has now solved this problem: The newly developed monochromator optics increase the photon flux in the tender energy range by a factor of 100 and thus enable highly precise measurements of nanostructured systems. *arö*



With the help of a new monochromator concept, nanostructures can be measured even more precisely. © HZB

Small Methods (2022): **Spectromicroscopy of nanoscale materials in the tender X-ray regime enabled by a high efficient multilayer-based grating monochromator.** S. Werner, P. Guttmann, F. Siewert, A. Sokolov, M. Mast, Q. Huang, Y. Feng, T. Li, F. Senf, R. Follath, Z. Liao, K. Kutukova, J. Zhang, X. Feng, Z.-S. Wang, E. Zschech, G. Schneider. **DOI: 10.1002/smtd.202201382**

UNRAVELLING TAUTOMERIC MIXTURES

Many (organic) molecules exist as a mixture of two almost identical molecules, with the same molecular formula but one important difference: A single hydrogen atom sits in a different position. In these so-called tautomeric mixtures, the two isomeric forms quickly merge into each other through the migration of individual atoms or groups of atoms and form a dynamic and sensitive chemical equilibrium. In their quantity ratio, the tautomers are constant among each other.

Tautomeric mixtures play a major role in biology: for example, many amino acids are tautomeric mixtures, and since they are building blocks of proteins, they may influence their shape and function and thus their biological functions in organisms. Due to the dynamic equilibrium, however, it is almost impossible to isolate the individual tautomers and determine their properties. Separating the electronic structure of such tautomeric mixtures from each other experimentally in a targeted manner has also not been possible so far. Classical spectroscopic methods "see" only the sum of the signals of each molecular form – the details of the properties of the two individual tautomers cannot be determined.

Breakthrough with RIXS at BESSY II

A team led by HZB physicist Alexander Föhlisch has succeeded in providing a method of experimentally unravelling tautomeric mixtures. Using inelastic X-ray scattering (RIXS) and a data processing/evaluation method newly developed at HZB, the individual proportions of the tautomers can be clearly deduced from the measured data.

Measuring a pure spectrum of each tautomer

"We can experimentally separate the signal of each individual molecule in the mixture by X-ray scattering, which leads to a detailed insight into their functionality and chemical properties," says Vinicíus Vaz Da Cruz, first author of the paper. "Specifically, we measure a pure spectrum of each tautomer, taking advantage of the element specificity and site selectivity of the method," Vaz Da Cruz explains. This allowed them to fully characterize the components in the tautomer mixture.

In the present study, the technique was applied to the prototypical keto-enol equilibrium of 3-hydroxypyridine in aqueous solution. The data were obtained at the EDAX terminal station at BESSY II.

New insights into biological processes

These results provide experimental evidence for concepts that have previously only been discussed theoretically in the literature. They are particularly interesting to enlighten and understand important biological processes such as the interaction between nucleoid bases of the DNA, metabolic conversion of fructose into glucose, or the folding of proteins.

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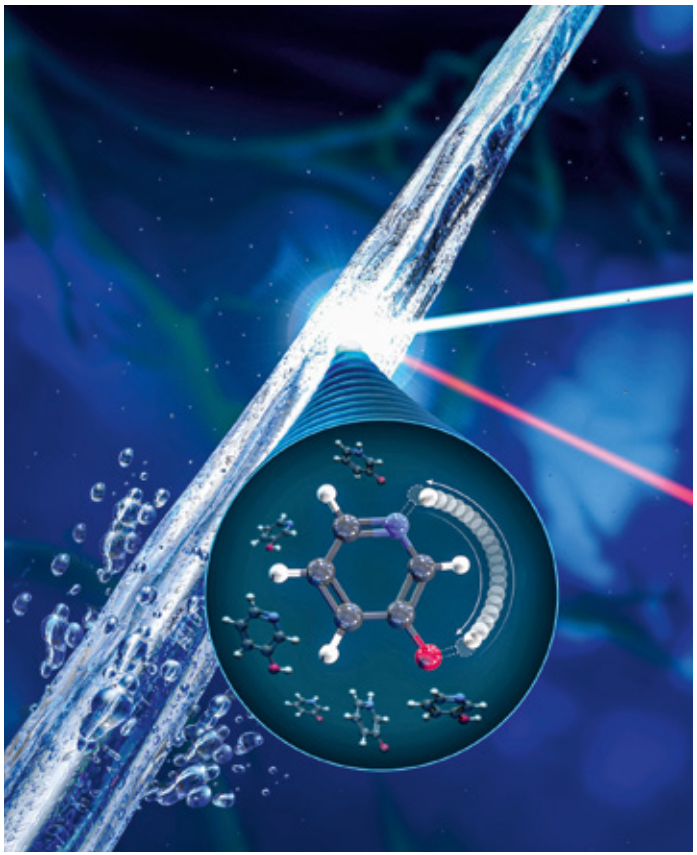


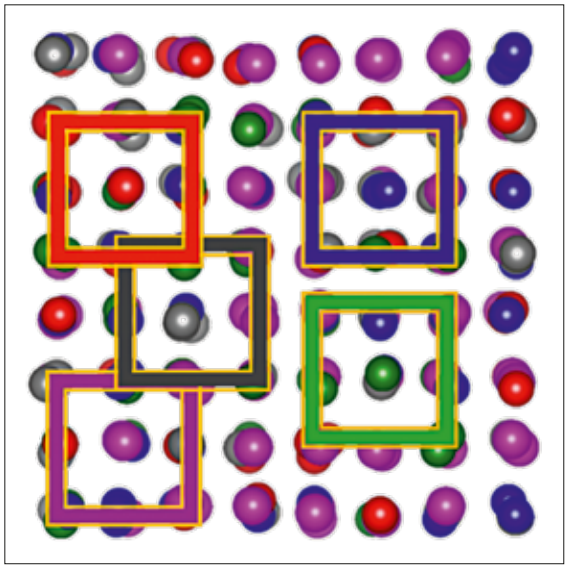
The illustration visualizes the experimental method, here on the prototypical keto-enol equilibrium.

© M. Künsting/HZB

The Journal of Physical Chemistry Letters (2022): Targeting Individual Tautomers in Equilibrium by Resonant Inelastic X-ray Scattering. V. Vaz da Cruz, R. Büchner, M. Fondell, A. Pietzsch, S. Eckert, and A. Föhlisch. **DOI: 10.1021/acs.jpclett.1c03453**

STRUCTURAL DISORDER AND MAGNETIC PROPERTIES IN HIGH ENTROPY ALLOYS

High entropy alloys or HEAs consist of five or more different metallic elements. Due to their heat and radiation resistance, they are an extremely interesting class of materials, for example, for coatings in reactors or in aviation. Since their macroscopic properties are strongly dependent on interatomic interactions, it is extremely interesting to probe the local structure and structural disorder around each individual element by element-specific techniques. At BESSY II, an international team led by HZB physicist Alevtina Smekhova has examined a so-called Cantor alloy – a model system to study the high-entropy effects on the local and macroscopic scales.



The Cantor alloy under study consists of chromium (grey), manganese (pink), iron (red), cobalt (blue), and nickel (green). X-ray methods allow to probe each individual component in an element-specific way.

© A. Kuzmin/University of Latvia, A. Smekhova/HZB

To investigate the local environment of individual components, the team used multi-edge X-ray absorption spectroscopy (EXAFS) and X-ray magnetic circular dichroism (XMCD). By conventional magnetometry, the scientists proved the presence of magnetic phase transitions and found some signatures of a complex magnetic ordering with a co-existence of different magnetic phases. "By probing the behavior of individual components at the atomic scale, we would gain valuable clues for the further development of new complex systems with the desired multifunctionality," says Smekhova. *arö*

Nano Research (2022): Local structure and magnetic properties of a nanocrystalline Mn-rich Cantor alloy thin film down to the atomic scale. A. Smekhova, A. Kuzmin, K. Siemensmeyer, C. Luo, J. Taylor, S. Thakur, F. Radu, E. Weschke, A. Guilherme Buzanich, B. Xiao, A. Savan, K. V. Yusenko, and A. Ludwig. **10.1007/s12274-022-5135-3**

POTENTIAL ENERGY SURFACES OF WATER MAPPED FOR THE FIRST TIME

Liquids are more difficult to describe than gases or crystalline solids. An HZB team has now mapped the potential energy surfaces of water molecules in liquid water under ambient conditions for the first time at the Swiss Light Source SLS of the Paul Scherrer Institute, Switzerland. This contributes to a better understanding of the chemistry of water and in aqueous solutions. These investigations are already being continued at the newly built METRIXS station at the X-ray source BESSY II. *arö*

Studies at the METRIXS station help to understand the chemistry of water. © unsplash

PNAS (2022): Cuts through the manifold of molecular H_2O potential energy surfaces in liquid water at ambient conditions. A. Pietzsch, J. Niskanen, V. Vaz da Cruz, R. Büchner, S. Eckert, M. Fondell, R. M. Jay, X. Lu, D. McNally, T. Schmitt, A. Föhlisch. **DOI: 10.1073/pnas.2118101119**

HIGHEST OXIDATION STATE OF RHODIUM DISCOVERED

Oxidation states of transition metals describe how many electrons of an element are already involved in bonds and how many are still available for further reactions. Teams from Berlin and Freiburg have now discovered the highest oxidation state of rhodium. This indicates that rhodium can contribute more valence electrons to chemical bonds than previously assumed. This finding could be important for understanding catalytic reactions involving rhodium.

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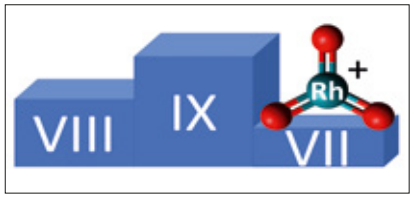


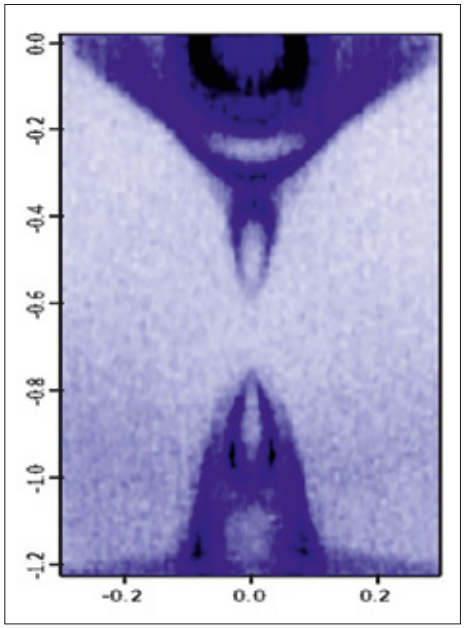
Its newly discovered oxidation state makes rhodium the chemical element with the third highest oxidation state ever, behind technetium and ruthenium.

© M. da Silva Santos et al.

Angew. Chem. Int. Ed. (2022): The highest oxidation state of rhodium: rhodium(VII) in $[RhO_3]^+$. M. da Silva Santos, T. Stüker, M. Flach, O. S. Ablyasova, M. Timm, B. von Issendorff, K. Hirsch, V. Zamudio-Bayer, S. Riedel, J. T. Lau. **DOI: 10.1002/anie.202207688**

NEW MAGNETIC SPLITTING EFFECT DETECTED AT BESSY II

Neodymium-Bismuth crystals belong to the wide range of materials with interesting magnetic properties. The Fermi surface which is measured in the experiments contains information on the transport properties of charge carriers in the crystal. While usually the Fermi surface consists of closed contours, disconnected sections known as Fermi arcs are very rare and can be signatures of unusual electronic states.



The experiment at the U125-2PGM undulator beamline of BESSY II shows bands with opposite curvature, so-called Fermi arcs. © HZB

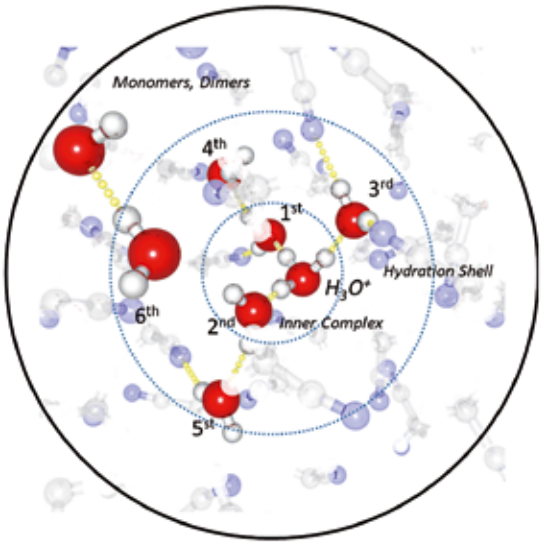
An international team of scientists has now presented experimental evidence for such Fermi arcs. They observed an unusual magnetic splitting in the antiferromagnetic state of the samples below a temperature of 24 Kelvin (the Néel-temperature). This splitting creates bands of opposing curvature, which changes with temperature together with the antiferromagnetic order. These findings are very important because they are fundamentally different from previously theoretically considered and experimentally reported cases of magnetic splittings. In the case of well-known Zeeman and Rashba splittings, the curvature of the bands is always preserved. Since both splittings are important for spintronics, these new findings could lead to novel applications, especially as the focus of spintronics research is currently moving from traditional ferromagnetic to antiferromagnetic materials.

arö

Nature (2022): **Emergence of Fermi arcs due to magnetic splitting in an antiferromagnet.** B. Schrunk, Y. Kushnirenko, B. Kuthanazhi, J. Ahn, L.-L. Wang, E. O'Leary, K. Lee, A. Eaton, A. Fedorov, R. Lou, V. Voroshnin, O. J. Clark, J. Sánchez-Barriga, S. L. Budko, R.-J. Slager, P. C. Canfield, and A. Kaminski. **DOI: 10.1038/s41586-022-04412-x**

HOW FAR CAN A PROTON MAKE ITS PRESENCE FELT WHEN EMBEDDED IN WATER?

A collaboration of research teams from the Max Born Institute, the University of Hamburg, Stockholm University, Ben Gurion University of the Negev and Uppsala University have obtained key insights into the electronic structure of hydrated proton complexes in solution. Using the novel liquid flatjet technology, they carried out X-ray spectroscopic measurements at BESSY II and combined them with infrared spectral analysis and calculations. This made it possible to distinguish between two essential effects: Local orbital interactions determine the covalent bond between the proton and neighboring water molecules, while orbital energy shifts measure the strength of the proton's extended electric field.

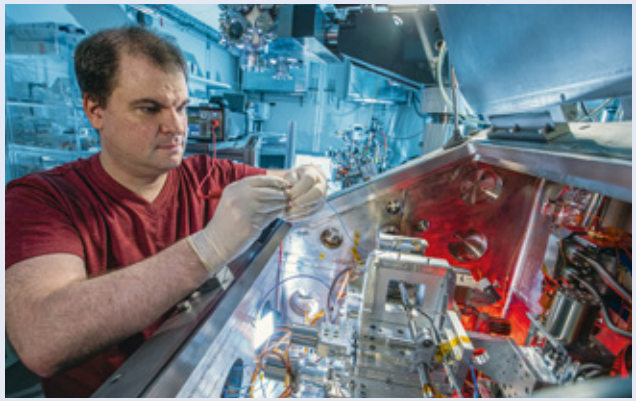


The spectral fingerprints of water molecules could be studied at BESSY II. The result: the electronic structure of the three innermost water molecules in an $H_7O_3^+$ complex is drastically changed by the proton. In addition, the first hydrate shell of five other water molecules around this inner complex also changes, which the proton perceives via its long-range electric field. © MBI

The results show: The proton interacts with three water molecules and forms an $H_7O_3^+$ complex. The hydrate shell of this complex is influenced by the electric field of the positive charge of the proton. These findings have direct implications for understanding proton hydration from protons in aqueous solution to proton complexes in fuel cells to water structure hydration pockets of proton channels in transmembrane proteins.

MBI/red.

Angew. Chem. Int. Ed. (2022): **From Local Covalent Bonding to Extended Electric Field Interactions in Proton Hydration.** M. Ekimova, C. Kleine, J. Ludwig, M. Ochmann, T. E. G. Agrenius, E. Kozari, D. Pines, E. Pines, N. Huse, Ph. Wernet, M. Odelius and E. T. J. Nibbering. **DOI: 10.1002/anie.202211066**



Climate-neutral: HZB strives for a climate-neutral society through science and innovation. For this reason, researchers at HZB are driving the discovery of energy materials at BESSY II and creating the basis for new sustainable technologies. © Silvia Steinbach/HZB

International and interdisciplinary: The synchrotron light generated at BESSY II is unique for research. That's why the facility receives around 2700 visits from guest researchers from all over the world every year. Researchers from a wide range of disciplines meet here.

© HZB

FACTS AND FIGURES ABOUT HZB

As of 31.12.2022

603

WoS, SCOPUS or Open Research Europe indexed publications were published by HZB scientists in 2022.

24.6

percent of HZB's 727 scientific staff were women at the end of 2022. In relation to the total number of 1,185 employees, the proportion of women was 31.6 percent.

183

doctoral students were supervised at HZB in 2022, with 23 dissertations completed at HZB.

79

percent of the beam time at BESSY II was used by external scientists at HZB in 2022.

295

days were dedicated to scientific use (including test operation for maintenance) of the storage ring facility BESSY II in 2022. It was available to users on 188 days. After the end of pandemic-related travel and work restrictions as well as safety requirements in the BESSY II experimental hall, the utilization rate, i.e. the proportion of time actually used by users for scientific experiments, rose to 96 percent.

240

cooperatives, including 67 international ones, were maintained by HZB with other scientific institutions at the end of 2022 – almost unchanged from the previous year (247).

33

adolescents and young adults were in seven different apprenticeships and three dual study programmes at HZB at the end of 2022. The proportion of women among the trainees was 36.4 percent.

26.87

million euros in third-party funding went to HZB in 2022. This included about 3.21 million euros from contract research, 5.46 million euros from services to third parties, about 8.92 million euros from project funding from the federal government and about 2.34 million euros from the European Union.

7

Young Investigator Groups were conducting research at HZB in 2022, four fewer than in the previous year. Of these Young Investigator Groups, six are part of the "Methods and Technologies for the Energy Transition" programme and one is assigned to the programme part "Quantum and Functional Materials".

87

new collaborations with companies were established by HZB in 2022 alone. This means that the total number of ongoing partnerships with industry fell slightly from 205 in the previous year to 194 now. Of these, more than 18 percent were collaborations with international partners and slightly more than 16 percent were joint projects with small and medium-sized enterprises.

2.78

million euros were received by HZB for technology transfer in 2022. Of this, 1.84 million euros came from infrastructure agreements and 941,000 euros from research and development partnerships with domestic and international commercial enterprises.

1,703

pupils experimented in the "Look into Matter" school laboratory in 2022. After the end of Corona-related restrictions, this is a significant increase compared to the previous year, when only 466 pupils were able to come.

7

patents were granted to HZB in 2022. HZB's patent portfolio comprised 156 patents at the end of 2022. 14 patents are the subject of ongoing licence agreements. For 13 invention disclosures from 2022, HZB and other technology experts are currently evaluating whether they can be patented and/or are commercially exploitable.

HZB signs Diversity Charter

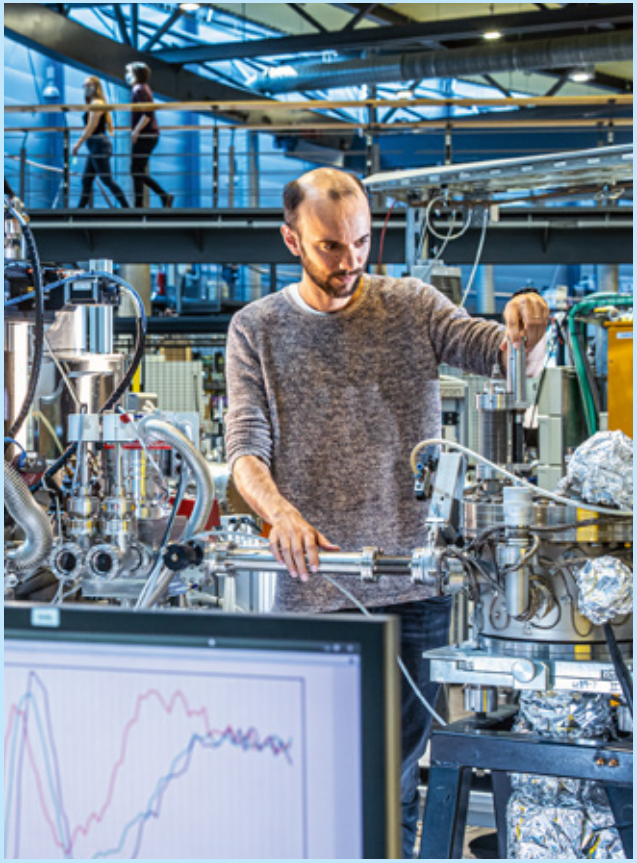
By signing the Diversity Charter, the HZB is once again setting an example for diversity.
© M.Setzpfandt/HZB

HZB has been a signatory of the "Charta der Vielfalt" (Diversity Charter) since February 2022. The Charta der Vielfalt association is the largest employer initiative to promote diversity in companies and institutions in Germany. The aim of the initiative, which was founded in 2006, is a prejudice-free working environment in which all employees – regardless of age, ethnic origin and nationality, gender and gender identity, physical and mental abilities, religion and world view, sexual orientation and social origin – are valued.

More than 4,900 organizations have signed the Diversity Charter to date. This means that the Diversity Charter represents over 15 million employees. "At the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), we promote diversity among our employees. It is an important prerequisite for the creativity and innovative strength of our research centre. Diversity is part of our working culture and brings different people together," says Thomas Frederking, Commercial Director of HZB.

40 years of research with synchrotron light in Berlin

In September 1982, the first electron storage ring officially went into operation in Berlin-Wilmersdorf under the name BESSY (Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung). In order to create this coveted synchrotron light, electrons are accelerated to near light speed in a circle. As they race around at this speed they emit special light, which scientists can use to look inside their samples. The successor facility in Berlin-Adlershof, BESSY II, is also based on this principle. It produced its first light beam in 1998 and is operated by Helmholtz-Zentrum Berlin (HZB). Presently, the facility receives around 2700 visits per year from guest researchers from everywhere in the world.



Research has been conducted with synchrotron light in Berlin for 40 years, since 1998 at BESSY II. © HZB

Since the first beam, the research possibilities with synchrotron light have expanded significantly. Today, experiments in which materials for an energy-efficient energy supply are researched play the most important role. The operation of the BESSY II accelerator is highly complex. To ensure that Germany and the world continue to benefit from synchrotron light beyond the next decade, HZB's accelerator specialists are working intensively with partners on the concept for a successor source, BESSY III.

In the CARE-O-SENE project, seven South African and German project partners are researching next-generation Fischer-Tropsch catalysts to optimize the production of sustainable kerosene on an industrial scale.

© care-o-sene.com

International Cooperation for sustainable aviation fuels

HZB and the South African industrial company Sasol will lead a consortium to develop and optimise next-generation Fischer-Tropsch catalysts. These play a key role for the production of sustainable kerosene on an industrial scale and thus for the long-term decarbonisation of aviation. The international research project CARE-O-SENE (Catalyst Research for Sustainable Kerosene) has received funding decisions of 30 million euros from the German Federal Ministry of Education and Research (BMBF). In addition, the industrial consortium partners are contributing 10 million euros.

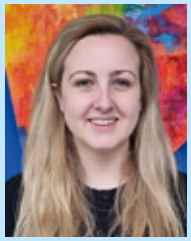
Unlike conventional kerosene derived from fossil feedstocks, so-called Sustainable Aviation Fuel (SAF) can be made from green hydrogen and sustainable carbon dioxide sources. The technology is intended to help decarbonise sectors such as aviation, as fossil fuels are particularly difficult to replace in this area. In addition to the HZB and Sasol Germany and Sasol Limited, other partners are contributing to the success of the project: The Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), the Karlsruhe Institute of Technology (KIT), the University of Cape Town (UCT) and INERATEC GmbH.

Appointments, awards and prizes

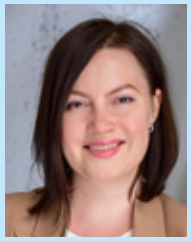
Professor Felix Büttner, who has led the Helmholtz Young Investigator Group MaXRay: Magnetism and Coherent X-ray Methods since 2020, has accepted an appointment to the W2 professorship in physics with a focus on coherent X-ray imaging techniques and magnetism at the University of Augsburg, effective 1 July 2022.

Professor Eva Unger was appointed W2 professor at Humboldt-Universität zu Berlin at the beginning of 2022. Unger leads a large team at HZB and develops scalable technologies for the production of perovskite semiconductors for low-cost and highly efficient solar cells.

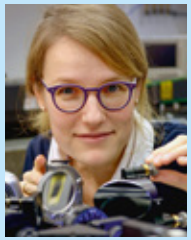
Professor Steve Albrecht was appointed to an S-W3 professorship at the Technische Universität Berlin in August 2022. At TU Berlin, he is head of the "Perovskite Solar Cells" department at Faculty IV Electrical Engineering and Computer Science. Through joint research, the next generation of highly efficient tandem solar cells is to be developed.



Dr Michelle Browne has started setting up her own Young Investigator Group at HZB in summer 2022. She focuses on electrolytically active novel material systems and aims to contribute to the development of next-generation electrocatalysts that can efficiently produce hydrogen.



Professor Olga Kasian, S-W2 Professor of "Materials for Electrochemical Energy Conversion" at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) since October 2021, was accepted into the Foundation's network on 20 June 2022 by the Werner-von-Siemens-Ring Foundation in recognition of her outstanding scientific achievements.



Professor Renske van der Veen was on the verge of completing the appointment process to an S-W2 professorship at TU Berlin at the end of 2022. Since the beginning of February 2023, she has been representing the field of "Dynamics in Light Energy Conversion" at the Institute of Optics and Atomic Physics there as part of a joint professorship with HZB.

Royal visit from Sweden

Visit of the Swedish delegation (from left to right): Thomas Frederking, Commercial Director HZB; Roland Sillmann, Managing Director WISTA Management GmbH; King Carl XVI Gustaf of Sweden; Per Thöresson, Swedish Ambassador in Berlin; and Bernd Rech, Scientific Director HZB.

© M. Setzpfandt/HZB

The Swedish King Carl XVI Gustaf and a group of business leaders from major corporations such as Ericsson, Nordholt, Vattenfall, ABB, Schneider Electric and Swedish representatives from the public sector and academia visited the Adlershof Technology Park on 11 May 2022. The science city in the south-east of Berlin is also home to the synchtrotron light source BESSY II operated by HZB.

During their visit to HZB, the delegation from the Royal Swedish Academy of Science and Engineering, which was also accompanied by the Swedish ambassador in Berlin, learned about novel photovoltaic technologies, the next generation of batteries and catalytic processes for the production and processing of green hydrogen. "The discussion with King Carl XVI Gustaf and his high-ranking delegation members on issues of energy supply based on renewable sources was very inspiring," says Professor Bernd Rech, Scientific Director of HZB. "We are very pleased about the many points of contact for increased cooperation."

HZB/Wista Management

OPENING OF THE HELMHOLTZ SESAME BEAMLINE HESEB

The synchrotron radiation source SESAME was opened in 2017. © SESAME

Since summer 2018, SESAME, the first large particle accelerator in the Middle East, has been generating brilliant synchrotron light. The acronym SESAME stands for Synchrotron-light and Experimental Science and Applications in the Middle East. The facility is located not far from the Jordanian capital Amman. It was founded under the auspices of UNESCO in cooperation with Egypt, Iran, Israel, Jordan, Palestinian Territories, Pakistan, Turkey and Cyprus.
The new Helmholtz SESAME Beamline (HESEB) was inaugurated there on 12 June 2022. It generates soft X-rays that enable research on a wide range of scientific questions, especially in solid-state, interfacial and surface physics. The element-specific interactions of soft X-rays with matter allow analytical investigations with high precision for many elements of the periodic table. “For many years now, SESAME has been demonstrating in an impressive way how a joint research project can bring people from different countries in the Middle East together for civilian research - a real bridge builder and a beacon of science diplomacy,” said Otmar Wiestler, President of the Helmholtz Association at the opening. The Helmholtz Association has funded the four-year HESEB project with 3.5 million euros. In addition to HZB, the Forschungszentrum Jülich, the Helmholtz-Zentrum Dresden-Rossendorf, the Karlsruhe Institute of Technology and DESY are involved in the project.

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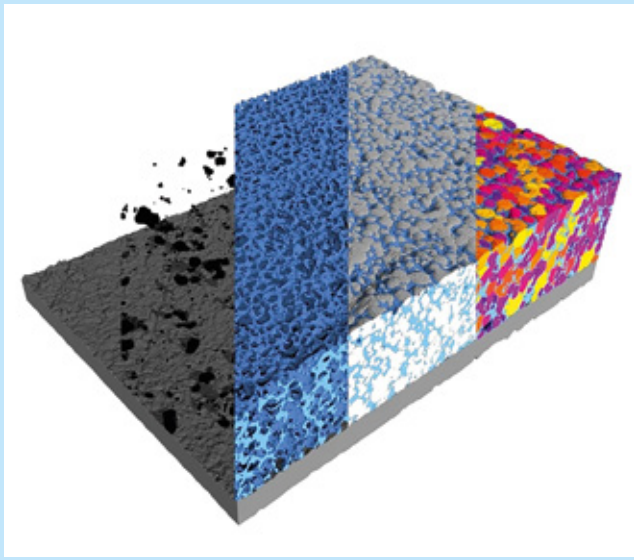
TOMOGRAPHY LAB FOR AI-ASSISTED BATTERY RESEARCH



X-ray tomography of a battery cathode, virtually disassembled into its components. © M. Osenberg, I. Manke/HZB/Binder/KIT

X-ray tomography allows a direct glimpse into a battery‘s inner structures during discharging and charging. “For example, when the lithium moves back and forth between the anode and cathode during charging and discharging, the lithium storage material may expand or chemical transformation processes may take place,” explains tomography expert and project coordinator Ingo Manke. The three-dimensional imaging of these structural changes can reveal weak points in terms of performance and durability, for example ageing processes.
HZB is now setting up an automated tomography laboratory that is specifically geared to the needs of solid-state batteries. The special feature: The 3D data of the charging and discharging processes (operando) can then be evaluated more quickly and in a more versatile way using artificial intelligence methods. The German Federal Ministry of Research and Education is funding the “TomoFestBattLab” project with 1.86 million euros. The combination of artificial intelligence methods and tomography measurement techniques is an innovative approach with a pilot function for equipping future laboratories. “The project helps us to digitalize battery research with regard to the requirements of Industry 4.0 and to accelerate the development of batteries,” says Manke.

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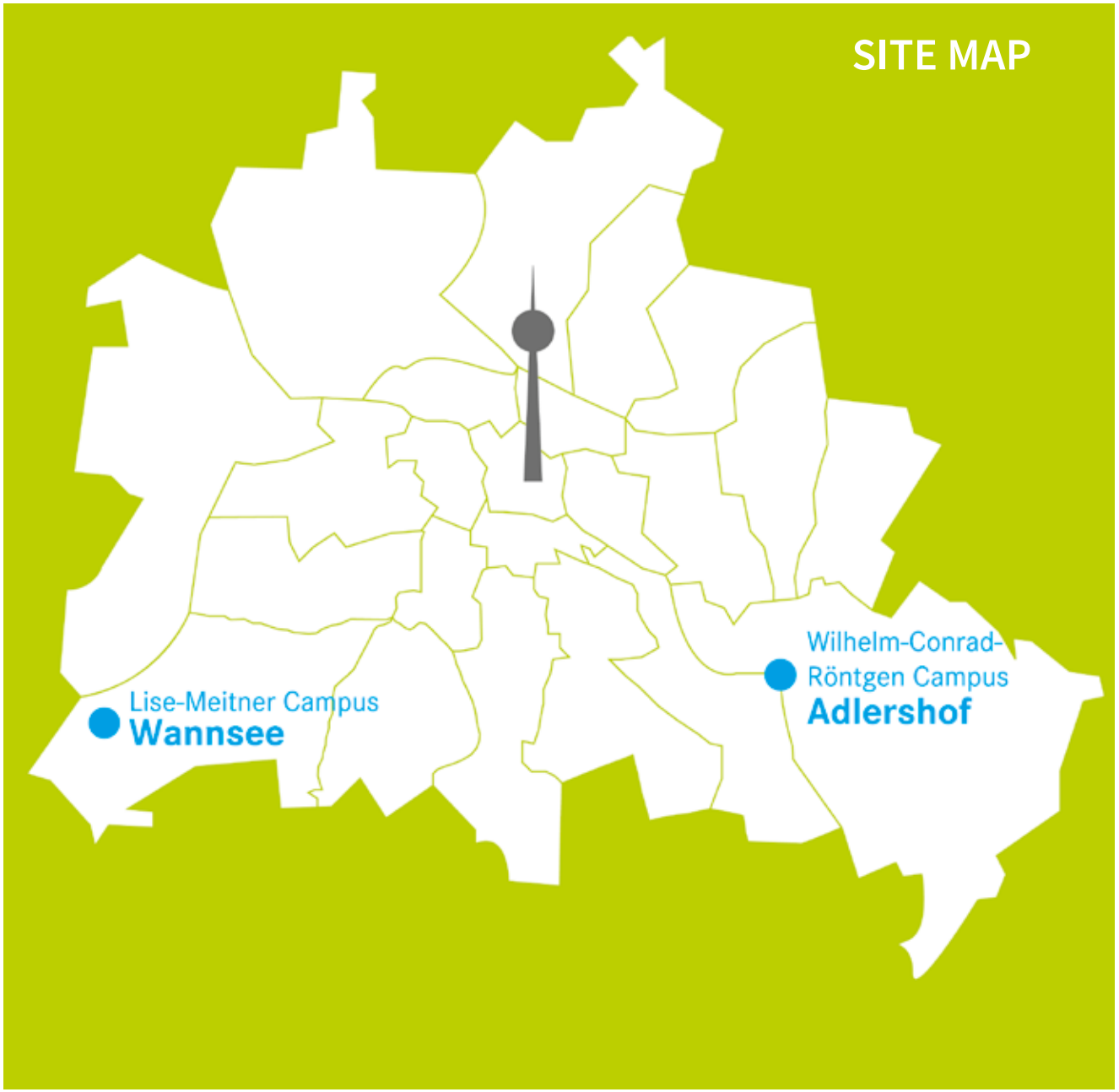

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HIGHLIGHTS FROM THE RESEARCH

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We are happy to keep you up to date on a monthly basis. For this you have two options: The **HZB-Newsletter (in German)** provides information about research at HZB, personnel news and dates. The **BESSY-News (in English)** is aimed at people who are particularly interested in research with synchrotron radiation, but also reports on the most important scientific news from HZB.

Please send an email with the subject: HZB-Newsletter and/or BESSY-News to redaktion@helmholtz-berlin.de.

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