HZB Helmholtz Zentrum Berlin

FOCUSSING ENERGY REALISING VISIONS

MOTOR RESEARCH

# ENERGY RESEARCH AT LARGE-SCALE FACILITIES

New solutions for the conversion and storage of solar energy

# THE HZB IN BRIEF

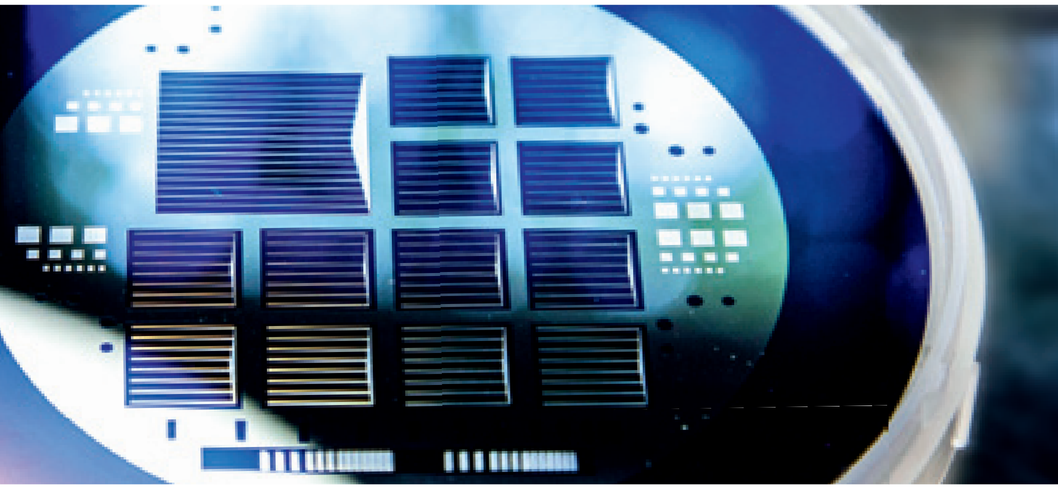
The Helmholtz-Zentrum Berlin (HZB) operates two large-scale scientific facilities for the study of the structure and function of matter: the BER II research reactor for neutron-based experiments and BESSY II, which is capable of emitting a special type of X-ray light called synchrotron radiation.

A major research emphasis is solar energy, with seven institutes and departments alone dedicated to its study. HZB scientists in these institutes and departments are conducting basic research to ensure that solar cells of the next several generations will be ready to hit the market. As such, they are working at developing new materials for **thin film solar cells** and for production of solar fuels. To make sure that new research findings quickly find their way into industry and application, the HZB, along with its partners, has established PVcomB, **the Competence Centre for Photovoltaics Berlin.**

In 2009, the HZB resulted from the merger of two Berlin-based research centers, each with its own rich history: the former Hahn-Meitner Institute and BESSY, the former Berlin Electron Storage Ring Society for Synchrotron Radiation. As a result of this merger, the HZB is one of only a handful of centers in the World with the set-up for **neutron-based experiments and synchrotron radiation** under one roof.

## Facts and figures

The HZB employs a staff of 1,100, 800 of whom are working at the Wannsee and another 300 at the Adlershof campus. The Centre's total budget is an impressive 110 million Euros. Beyond Berlin and the neighboring state of Brandenburg, the HZB's many collaboratives include some 400 partners at both German and international universities, research facilities, and private companies.



Researchers are investigating new materials and architectural ideas for solar cells at the HZB's two large-scale facilities.

# PROMOTING SOLAR ENERGY

**The energy transition is an undertaking of gigantic proportions: The plan is that by 2020, renewable energy sources constitute roughly 35 percent of Germany's total energy consumption – and as much as 80 percent by 2050. This goal is attainable and solar energy will make an important contribution towards it.**

The reason behind this optimism lies with Germany's existing research infrastructure. Research into solar energy conversion is a far cry from being finished. Quite the opposite: It delivers many alternatives to conventional solar cells made from crystalline silicon wafers whose manufacture consumes a lot of energy. Specifically, **thin film solar cells** that are silicon-based or made from other semiconductor materials have tremendous potential: Their efficiency can be increased and the material and energy investment decreased during production. There is an **unmet need for research** into materials and components for energy storage like solar fuels or fuel cells.

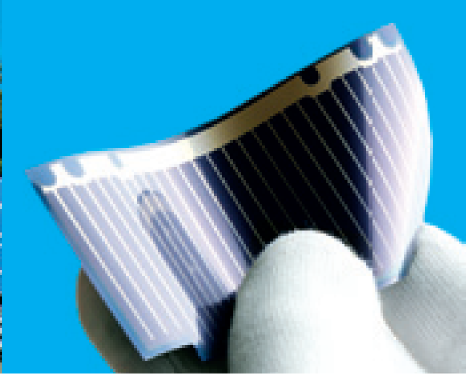
The Helmholtz-Zentrum Berlin is a European leader in solar energy research[1]: We have put together an extensive research infrastructure to allow for a deep and accurate look at matter. Specifically, it enables us to look at processes and quantum physics effects that define material properties. A deeper understanding of these processes is key to developing and systematically testing new ideas.

## The sun's potential

Although more than 1,000 watts per square meter make it to Earth's sun belt, Germany, located in Earth's more Northern latitudes is only able to harvest some 600 watts per square meter on a sunny day. Yet even in this densely populated industrialized nation, solar radiation exceeds total energy consumption by a factor of 80[3].
In Germany, top-performing 30-gigawatt photovoltaic modules were installed in mid-2012. During the first half of the year, photovoltaics covered around five percent of gross energy consumption[4].



1 According to the 2009 Elsevier Ranking
2 FVEE 2013 Research Goals, p. 11
3 Source: www.bmu.de/erneuerbare_energien/kurzinfo
4 Gross energy consumption in Germany approx. 625 TWh per annum (BMWi)



The cost of PV modules has gone down by a factor of ten over the last 25 years[2]; at this point, “grid parity” has been reached and isolated solar energy consumption is already profitable.

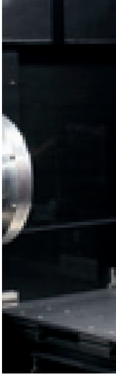
Research is working on developing next-generation solar cells including flexible CIS solar cells on titanium foil.

# DOING RESEARCH AT LARGE-SCALE FACILITIES

At the HZB’s Wannsee campus, researchers are using the **BER II neutron source** to glean insights into atomic processes as they occur within materials. **BESSY II, Berlin’s electron storage ring,** has the necessary capabilities for a large number of microscopic and spectroscopic methods. Here, researchers are able to examine the formation of crystalline layers and interfaces to learn about the effects a material’s atomic or molecular structure has on its electronic properties. Both large-scale facilities are continuously fine-tuned and have the reputation for being global leaders in their field.

High-end basic science research requires a lot of patience to produce the basic requirements for an unending **source of true innovation.** In the case of BER II and BESSY, we have exceptional tools right at our fingertips. With their help, we are able to examine how we can utilize solar energy using complex materials. Yet the HZB’s research spectrum encompasses not only basic science research but also multiple application-relevant questions we as partners for industry are promoting in the context of the PVcomB center of excellence.

The sun radiates some 10,000 times more energy to Earth than mankind currently has use for.



Experienced HZB researchers mentor both German and international users.

# DEEP INSIGHTS INTO MATTER

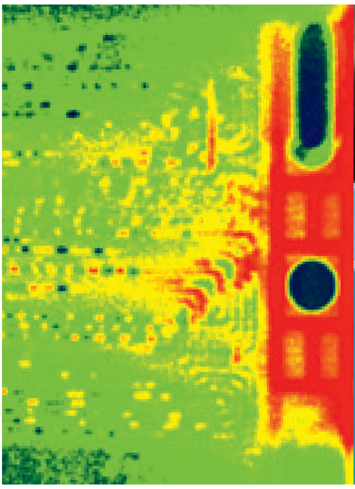
## AFTER THE BER II MODERNIZATION

Up to five times the amount of neutrons per experiment – remodeling Berlin-based research reactor BER II has definitely been worth it. New neutron conductors and new components in the neutron source's interior ensure that, since March 2012, BER II users are met with optimal conditions and are able to conduct top-notch scientific experiments using one of 15 total available measuring stations.

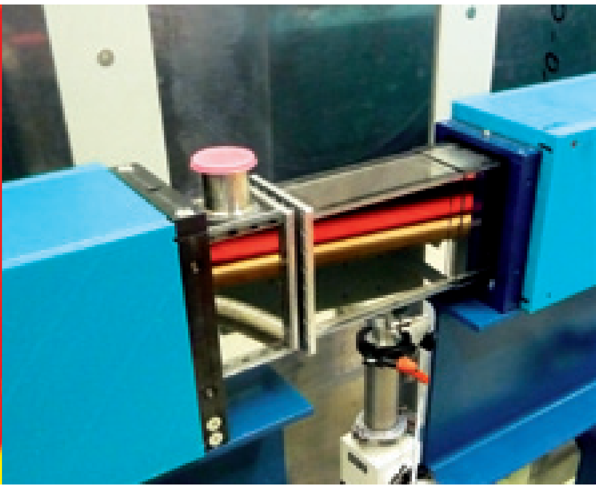
In terms of energy research, some of the techniques of neutron diffraction and radiography are especially useful. As such, **neutron tomography for visualization** allows for an examination of solidly constructed fuel cells during operation and observe how the water that is produced in the process diffuses within the fuel cell and subsequently drains away. Such insights are important in that they help improve fuel cell efficiency.

Semiconductor materials like those used in thin film solar cells can be studied using high-resolution powder-diffractometers with the help of **neutron diffraction.** Theoretical deliberations have shown that tiny disturbances within the crystalline structure known as point defects barely compromise a thin film cell's electronic properties. Yet a detailed analysis of the concentration of point defects in copper-based thin film solar cells

With neutron tomography at BER II, researchers are able to observe how water produced within a fuel cell is distributed while the cell is operating.



New supermirrors limit neutron loss so that users benefit from a stronger neutron flow.



HZB experts have made extreme sample environments including low temperatures and strong magnetic fields available for superconductor research.

(called chalkopyrites) has not yet been performed. Here, neutron diffraction revealed that high concentrations of copper defects exist in the materials that were being examined: Within the crystal grid, several locations were identified where a copper atom was missing. It seems odd yet is reassuring that in spite of a large number of defects these kinds of solar cells are still perfectly functional.

## Neutrons bring light into the dark

A staple in energy research is the superconductivity phenomenon. Current substances lose their electrical resistance only at temperatures that are well below freezing and as such must be cooled to a temperature of negative 196 degrees Celsius using liquid nitrogen. If materials capable of conducting electricity at room temperature without a loss of charge could be developed, this would translate into substantial savings in terms of transport of electric current. Researchers are able to experimentally test new hypotheses about key factors surrounding superconductivity at the BER II neutron source and, based on the insights gleaned from these experiments, **more purposefully develop new superconducting materials.**

## Neutron research upgrades

- The new cooling source delivers a >1.5-fold increase in neutron flow
- The neutron conductors' new supermirror coating delivers an amplification factor of 4-8
- Several instruments were converted and optimally positioned
- A unique high field magnet capable of delivering up to 25 Tesla for neutron diffraction experiments is currently under construction

At each of the 50 beamlines, researchers are able to screen their samples using synchrotron radiation.

# BESSY II – A MICROSCOPE FOR SPACE AND TIME:

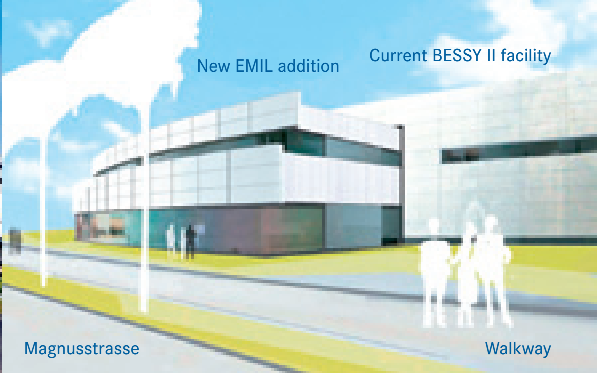
At the Adlershof campus, Berlin's electron storage ring BESSY II delivers intensive synchrotron light at frequencies ranging from a few terahertz to the visible spectrum all the way to hard X-rays. With its help, atomic and molecular processes that take place within organic and inorganic materials can be examined at a **spatial resolution on the order of nanometers** (i.e. a billionth of a meter). In addition, ultrashort pulses of synchrotron radiation allow for insights into the dynamics of high-speed reactions on the order of femto seconds ($10^{-15}$ seconds), for example at the interfaces in new thin film solar cells.

Synchrotron radiation is emitted by electrons that are beamed into the storage ring at near the speed of light and then kept in orbit. In the process, they tangentially emit photon packets, or pulsed light. Germany's BESSY II is the leading third-generation synchrotron radiation source in the soft X-ray range. Each year, it attracts some 2,000 scientists from Germany and abroad, all of whom appreciate BESSY's exceptional reliability and stability. At each of the more than **50 separate beamlines,** researchers are able to individually set up photon wave length, polarization, and energy. Experts are constantly at work fine-tuning the HZB's large-scale facilities and now, thanks to the new top-up mode and fast orbit feedback, have created optimal conditions for ever more sensitive measurements.

www.light2hydrogen.de

## ISSIS to BESSY II: Catalysts for hydrogen production from sunlight

At BESSY II's ISSIS beamline, Fritz-Haber Institute scientists are working with HZB experts and other partners to glean new insights into the efficiency of catalysts. As part of the BMBF funded excellence initiative "Light2Hydrogen," they are studying new kinds of photocatalysts that consist of polymeric carbon nitride and photoactive semiconductors like chalkopyrites and silicon. These material systems are capable of using sunlight to split water into hydrogen and oxygen.

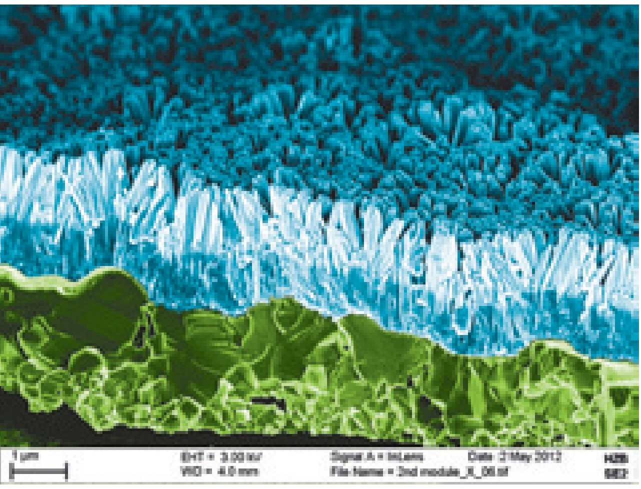



Starting in 2015, energy research will benefit from new opportunities at the EMIL laboratory.

## EMIL: Research involving energy materials

With EMIL (Energy Materials In-Situ Laboratory Berlin), the Helmholtz-Zentrum Berlin and the Max Planck Society (MPG) are together setting up an internationally unparalleled laboratory at BESSY II, which, starting in 2015, will offer new options for research involving energy and catalytic materials.

SISSY, the Solar Energy Materials In-situ Laboratory at the synchrotron source, is one of EMIL's central aspects. With direct access to a BESSY II storage ring beamline, EMIL offers unparalleled options for **X-ray analytics.** A major advantage is the fact that the solar cells no longer have to be transported from the lab to the measuring station to be examined but instead are prepared on location and "in system" in the "cluster tool" without upsetting the vacuum. This prevents the surfaces and interfaces from coming into contact with the air and being contaminated. The intent is to conduct these kinds of experiments while the film is growing so that you will basically be able to follow the formation of the layer's properties "live." For the first time ever, hard and soft X-rays are available for purposes of this kind of analysis in a lab setting. One part of the lab, called CAT, is set aside for the examination and optimization of catalytic processes that play a role in energy storage.



This scanning electron micrograph shows an absorption layer that was combined with zinc oxide nanorods, which allows the solar cell to trap more sunlight.

# NEW THIN FILM OPTIONS

## Kesterite ($Cu_2ZnSnS_4$) as a photovoltaic absorbent

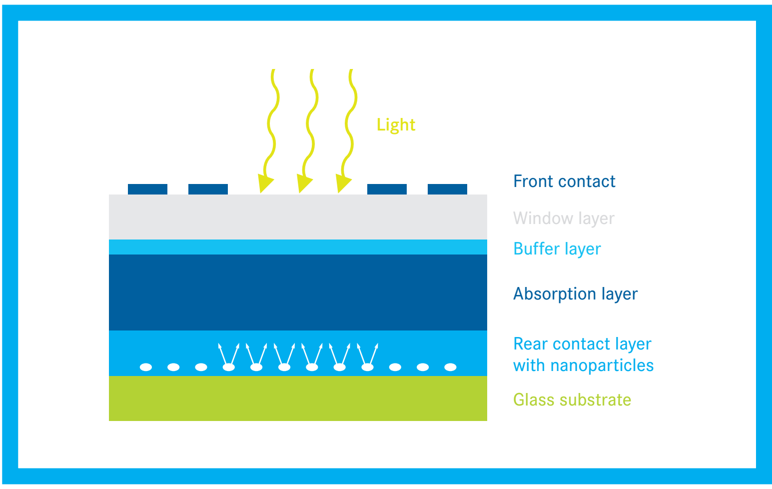
It‘s true that high-efficiency thin film solar cells like chalkopyrite cells are capable of reaching efficiencies in excess of 20 percent while containing rare elements like indium and gallium. It is precisely these elements that, in the kesterite layer, are replaced with the much more common elements zinc and tin. This is why kesterite cells can be the interesting option as inexpensive solar cells despite the fact that, at 10 percent, their efficiency is rather low.

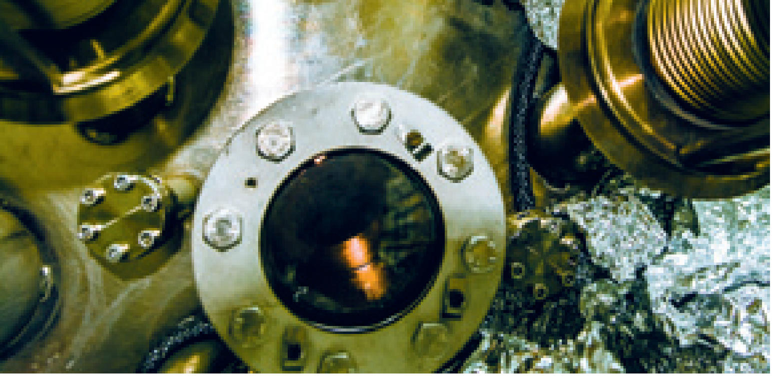
Now, Prof. Dr. Marcus Bär‘s Helmholtz University Future Researchers Group has documented how the electronic interface structure‘s kesterite and adjacent buffer layer don‘t fit together: There is a “banding mismatch” that clearly limits efficiency.

In the case of the chalkopyrite cells it‘s taken almost 30 years of continual optimization for them to become highly efficient. The plethora of methodologies available at the HZB now allows for deeper insights that can be notably speed up through optimization of kesterites and other material systems.

### Modern-day thin film solar cells

**Thin film solar cells consist of multiple layers, each of which performs an important function and is thus capable of increasing efficiency. Here, the incoming sunlight produces electron-hole pairs in the absorption layer - at the p-n junction between two oppositely doped semiconductor materials - that drain in the form of current via the contacts. The buffer layer, which may consist of cadmium sulfide, improves the solar cell’s properties. Researchers are experimenting with additional layers including a layer of metallic nanoparticles shown here, that reflect part of the light onto the absorption layer for a larger portion to be converted.**





In ultra-high vacuum apparatuses, solar cells are coated and examined.

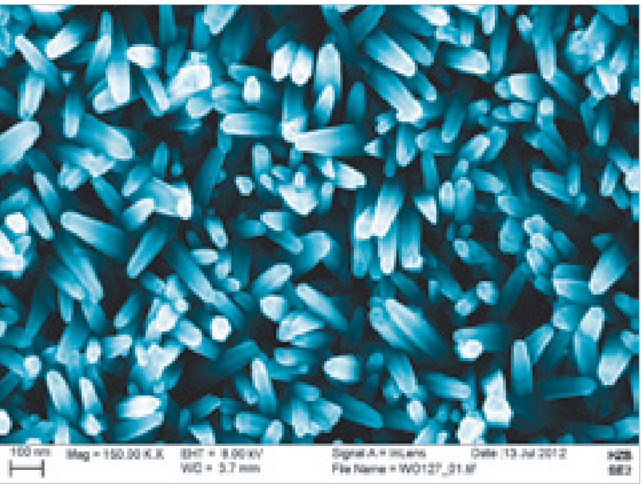
## Chalkopyrite nano-optical solar cell architecture

Chalkopyrites have properties that are ideally suited to solar cells. They reach their maximum efficiency below polycrystalline thin film solar cells. Unfortunately, the materials they use like indium are rather expensive. Which is why it’s important to make the chalkopyrite thin films even thinner without compromising their efficiency – because a thin film absorbs that much less sunlight.

Which is why Dr. Martina Schmid, head of the HZB’s future researchers group, and her team are hard at work using **nano-optical solar cell architectures:** Here, metallic nanoparticles are found below the ultrathin chalkopyrite film. These nanoparticles diffract light that would otherwise disappear in the photovoltaic cell’s rear wall without being reflected back onto the chalkopyrite layer. Using the material composition and the form and size of these nanoparticles, the researchers are able to influence which of the wavelengths of light are ultimately diffracted.

Another idea involves integrating a layer consisting of tiny micro lenses and capable of focusing light onto tiny chalkopyrite islands into the solar cell architecture, which means that the material between the islands could be saved.

**An animation showing the way a solar cell works can be found on the HZB’s YouTube channel at:** www.youtube.com/user/hzbkanal



This electron micrograph clearly shows the metal oxide rods sticking out from the layer like the fibers of a rug.

The “integrated system” allows for a large number of different measuring protocols.

# OBSERVING AND CHECKING GROWTH

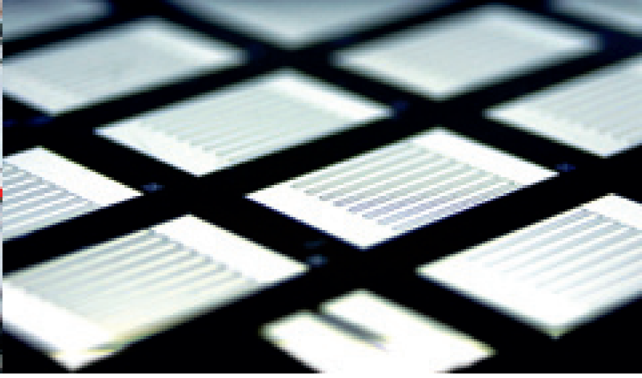
The structure of efficient thin film solar cells is complex, consisting of multiple layers of different semiconductors each of which plays an important role and contributes to the cell’s ability to efficiently convert sunlight to electricity. The processes that take place within, between, and at the surfaces can be influenced and optimized through the manufacturing process. The experiments at the BESSY II beamlines generate the knowledge that is needed for purposeful thin film technology development.

The electronic and optical properties of semiconducting thin films are apparent as early as at the time of their growth on a substrate. Which is why the **design of the growth process** is a key determinant of high-efficiency thin film solar cells. The BESSY II beamlines allow scientists to observe and analyze these growth processes “in situ” - in other words in real time. To this end, they are using high-temporal-resolution X-ray diffraction and fluorescence.

As such, Dr. Roland Mainz and his colleagues are able to observe whether elements from adjacent layers or from the surrounding atmosphere are incorporated into the growing film or whether they evaporate from the film’s surface and which crystalline compounds result from this process. At the same time, they are also able to determine the particle size in the fully crystallized regions. And they are also able to see where mechanical tensions arise within the layers.

## ILGAR-based improvement to CIS modules

HZB scientists at the Institute for Heterogeneous Materials Systems have developed the ILGAR method (Ion Layer Gas Reaction) to produce buffer layers made from indium sulfide or zinc sulfide/indium sulfide. These are meant to replace the cadmium sulfide buffer layers that are normally used in thin film solar cells. In addition, it does away with an environmentally hazardous deposition protocol. The solar cells thus produced reached efficiencies of over 16.1 percent – well above the efficiencies that were previously reached with the indium sulfide buffer layers.



In back wall solar cells, all contacts are placed on the side facing away from the sun so as to avoid the casting of shadows.

At BESSY II's EDDI beamline, the researchers developed two measuring chambers to allow for the study of these kinds of processes under conditions resembling those of industrial production. As such, they were able to optimize the manufacturing process for Cu(In,Ga)$S_2$-cells so that their efficiency was able to reach a new record high.

## Back wall solar cell with silicon hetero contacts reaches record efficiency

The back contact heterojunction solar cell unites all of the benefits of two different photovoltaics technologies: back contacts and silicon hetero contacts. Here, the metal fingers used to collect electricity are located on the cell's rear wall so they don't cast a shadow on the cell. The hetero contact technology involves two semiconductors with different gaps in their banding used within the same solar cell, in this case crystalline and amorphous silicon.

Both protocols have the advantage that they can be used industrially: Combining the two allows for very high (approx. 25%) efficiencies to be reached. In a jointly funded project by the German Federal Ministry for the Environment and the companies Bosch, Schott Solar, Sunways, and Stiebel Eltron, HZB researchers together with their colleagues at the Institute for Solar Energy Research Hameln (ISFH) are continuing to develop this new type of solar cell. In the process, they have scored a major success: Up until 2011, the efficiency was still at 15 to 16 percent; now it's at 20.2 percent.

A researcher in the process of preparing a sample using the ILGAR method.

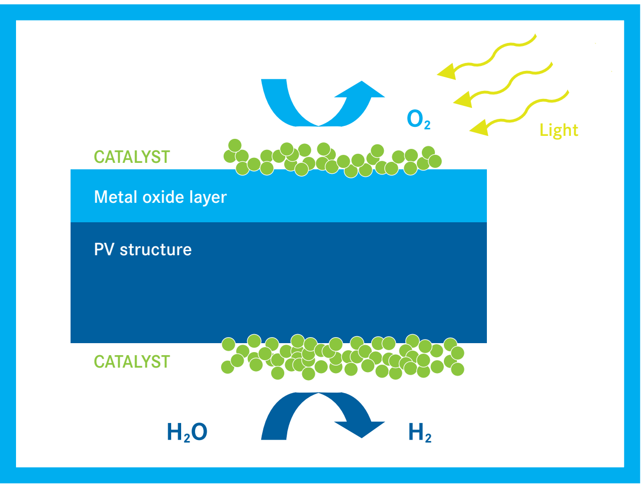
This thermogravimetric analysis facility allows for the study of the thermic behavior of catalysts in different gaseous atmospheres.

# SOLAR FUELS STORE ENERGY FROM THE SUN

At the HZB's Institute for Solar Fuels, Prof. Dr. Roel van de Krol and his team are developing and studying new material systems capable of converting solar energy into chemical energy for ease of subsequent storage as efficiently as possible. Their work is based on an electrolytic process with whose help water can be split into its components oxygen ($O_2$) and hydrogen ($H_2$). $H_2$ is a chemical storage molecule for solar energy: The energy stored inside a fuel cell can be used to generate electric current. Hydrogen, however, can also be processed further into solar fuels, including methane, methanol, and even gasoline or diesel.

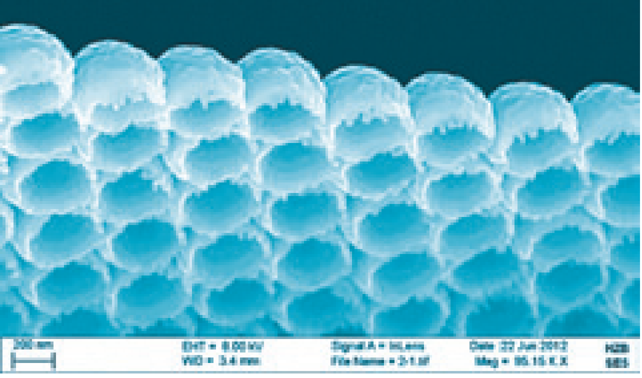
**Here, the HZB's considerable expertise in the area of solar cell research is essential:** To ensure that the splitting of the water molecules works, light has to first generate tension inside the electrode – like it does in a solar cell.

The electrode's core consists of a multitude of oppositely doped semiconductor layers that form multiple junctions (known as a tandem configuration). Originally, a minimum of three such junctions were required, each of which was made up of three separate layers. By now, the researchers have shown that one of these junctions can be replaced by a film of metal oxide. This is one way for simplifying production of these multi-layer systems, increasing their chemical stability against corrosion by water, and, at the same time, improving their efficiency:




**Integrated photoelectrode with many talents**

This electrode integrates absorption layers from photovoltaically active semiconductor structures, a metal oxide film, and catalysts. The electrode is submerged in water. Incoming light produces a current that splits the water molecules into their oxygen ($O_2$) and hydrogen ($H_2$) component parts. The catalysts at the electrode's surface help further accelerate this process. The hydrogen gas that is produced is drained and can subsequently be stored or worked on further using conventional technologies.



Nanostructures, made from iron oxide here, can also take the shape of hollow spheres.

For while the semiconductor junctions are using especially long-wave red light for charge separation, the metal oxide layer is able to convert light’s blue wavelengths into electric current.

The complex material system comprised of light-absorbing layers is coated with catalyst particles that notably increase the yield of hydrogen gas.

The researchers are already working on the next stage to obtain more hydrogen gas from solar energy. They are experimenting with **metal oxide nanostructures as a single layer of metal oxide** does not make for optimal results: For one, they have to be thick enough in order to absorb enough light, for another, as they should be thin enough to allow for the charge carriers’ proper drainage. Nanostructures offer many interesting solutions: A thin nanorod “carpet” means short distances for the charge carriers to travel but also sufficient distances for light absorption. In addition, the “carpet fibers” have a huge surface that can be coated with catalyst particles. This would further increase the hydrogen yield.

Synthetic monocrystals of $CuInS_2$ (above left), $TaS_2$ (below left), or $PtS_2$ (right) can be used as starting substances for catalysts. But researchers are now also working with far less expensive materials.

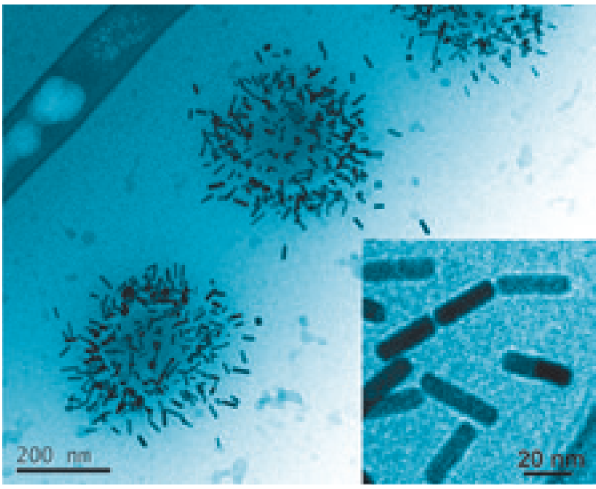
An expertise in chemistry, growing crystals, and materials science are prerequisites for producing samples using new kinds of material systems.

## New materials for catalysts

New optically active catalyst materials can greatly increase efficiency during the energy conversion process. Since platinum catalysts are very costly, HZB researchers are working on inexpensive alternatives that possess an especially extensive “active surface.” This can be done, for example, using **catalytically active nanoparticles** embedded within some kind of carrier material.

HZB Chemist Dr. Yan Lu of the Institute for Soft Matter and Functional Materials is working on synthesizing nanoparticles with custom-made optical properties. Lu’s nanoparticles consist of a gold core surrounded by one or several shells of metal oxide particles. The gold core “harvests” light’s electromagnetic energy and uses it to stop undesirable processes.

By now, Lu and her colleagues have successfully produced nanoparticles with different properties. The shape of the metal oxide particles that surround the gold core play a key role in all this: They can be spherical or elongated or be layered onto the gold core at different densities. With the help of BESSY II’s X-ray microscope, the researchers are currently investigating the particles’ structure and measuring their optical and electronic properties using spectroscopic methods.




These nanoparticles consist of gold nanorods immobilized in a bowl made from thermosensitive polystyrol.

Employees are testing a new coating option at the PVcomB's sputter facility.

# PVcomB – ALWAYS ONE STEP AHEAD

In photovoltaics research, PVcomB is a link between basic science research and industrial application: The goal is to take research findings that have come out of institutes like the HZB, Berlin Technical University, and the University of Applied Sciences for Technology and Business (HTW) and continue to develop them into technologies with real-world applicability.

The PVcomB has to always be one step ahead working on topics today that will become relevant at some point down the road. This goes for the efficiency with which solar cells convert light to electricity, for example. Labs everywhere are working at optimizing efficiency. The competition is stiff in this field, which is why the PVcomB is charting new territory. Currently, solar cells are still coated using thin, two-dimensional films. At the PVcomB, researchers are developing **technologies with whose help the layers can be made to grow** with purpose so that they turn into three-dimensional structures as is already the case at the HZB in basic science research.

System optimization is also important: Solar cells should not be considered in isolation - they are influenced by external factors and also influence them in turn. Which is why the PVcomB is dedicated to the importance of solar cells in systems – in order to make inferences for the thin film photovoltaics of the future.

www.pvcomb.de

## The PVcomB:

- supports industry partners with setting up new lines of production
- continues to develop industrial processes
- explores new and promising high-risk concepts
- transfers results from basic science research and converts them to the PVcomB's standard 30 by 30 $cm^2$ size
- operates its own lines of reference as benchmarks for process control
- collaborates with the university system to ensure that current course offerings are in line with the current state of research and application
- creates teaching positions that are in line with unmet needs in the real-world setting

Left: Students engrossed in an experiment performed in the school laboratory. Right: A young researcher checks an experimental setup.

# ACTIVELY ENCOURAGING THE NEXT GENERATION

The HZB offers interested students, graduates, university students, PhD students, and postdocs many opportunities for learning and furthering their qualifications.

## Good prospects for students

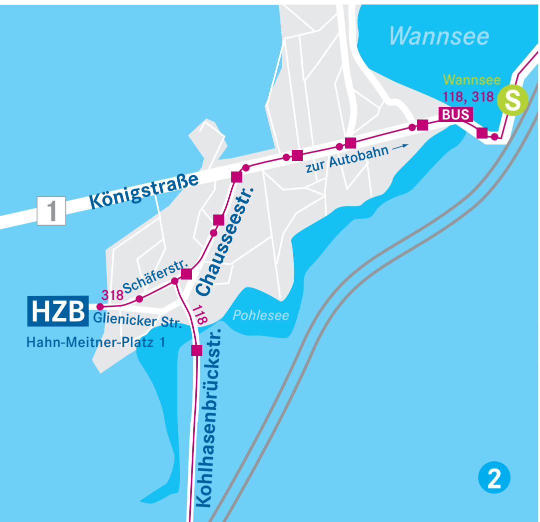
The HZB collaborates closely with universities in Berlin and Brandenburg. Many senior HZB researchers hold teaching appointments at these institutions and mentor and supervise students during the research and thesis-writing process. Each year, the HZB offers a ten-day neutron scattering course, an international school for photovoltaics, and an eight-week, comprehensive **summer school.** These programs are a good opportunity for students to familiarize themselves with lab work and with HZB's large-scale facilities.

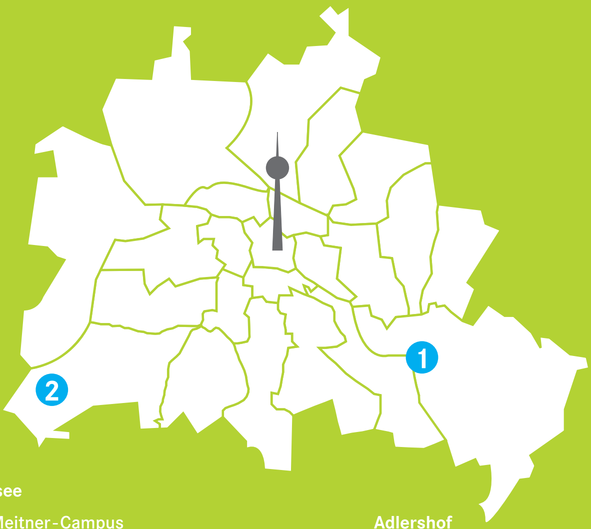
## Hands-on science

In the 'Blick in die Materie' student lab, students are able to delve into the fascinating world of physics while learning about the job of a researcher in a playful way. Teenagers who are interested are able to get a taste of real life at the HZB as part of the Centre's internship program.

### A successful start into professional life

Teenagers are also given the chance of being trained in a forward-looking line of work like administration, mechanical engineering, IT, or environmental and radiation protection.

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