

FOCUSSING ENERGY REALIZING VISIONS



## **BESSY II FORESIGHT WORKSHOP ON ENERGY MATERIALS RESEARCH**

October 10 - 11, 2016  
Berlin-Adlershof



Dear participant,

The Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) kindly welcomes you to its foresight workshop on Energy Materials Research.

Modern societies are facing the urgent global challenge of a growing demand for energy and the sustainability of its supply. Meeting this challenge requires a tremendous effort in research, innovative solutions and smart applications. At the same time, however, it provides enormous opportunities in developing new processes and technologies for applications by entrepreneurs and industry.

Scientists from around the world have accepted the task to develop and refine new scientific concepts and technologies to pave the way to clean and sustainable energy supply of tomorrow. HZB has taken up the challenge of developing advanced materials for energy conversion and storage as well as energy-efficient information technologies. With its research, HZB aims at contributing to a sustainable, economic and secure energy supply. Relying on its portfolio of dedicated laboratory infrastructures that allow guided materials design, synthesis and analysis, HZB targets the full chain from the discovery of basic principles in energy materials to the transfer of results to applications for the society.

One of the infrastructures at BESSY II is EMIL@BESSYII, the Energy Materials In-situ Laboratory. In a concerted effort together with the Max Planck Society, EMIL@BESSYII will offer a pivotal, unique infrastructure for Energy Materials Research at HZB's synchrotron light source. In addition to EMIL@BESSYII, a variety of dedicated experimental set-ups at BESSY II allow experiments on energy materials for applications in photovoltaics, energy conversion, energy storage and energy saving.

We invite you to discuss the challenges and opportunities for Energy Materials Research in general and at current and future synchrotron light sources with us at the workshop.

This workshop is the sixth in a row of Foresight Workshops, which are designed to foster and extend a discussion platform for future projects and research activities in concert with current and future users of BESSY II. A good part of our speakers and participants does not (yet) use synchrotron radiation for their research; in particular their input is of paramount interest for a dialogue to identify future scientific tasks as well as expectations, needs, and requirements for cutting edge science with synchrotron radiation. This will define challenges for us to take up in order to meet the requirements of our scientific communities.

We hope that this workshop will stimulate your interest in future developments at BESSY II, initiate fruitful discussions, new experiments and collaborations. Thank you all for joining us and enjoy the meeting.

Sincerely,



Prof. Dr.-Ing. Anke Kaysser-Pyzalla  
Scientific Director and Chief Executive



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# Workshop on Energy Materials Research 10./11.Oct.2016

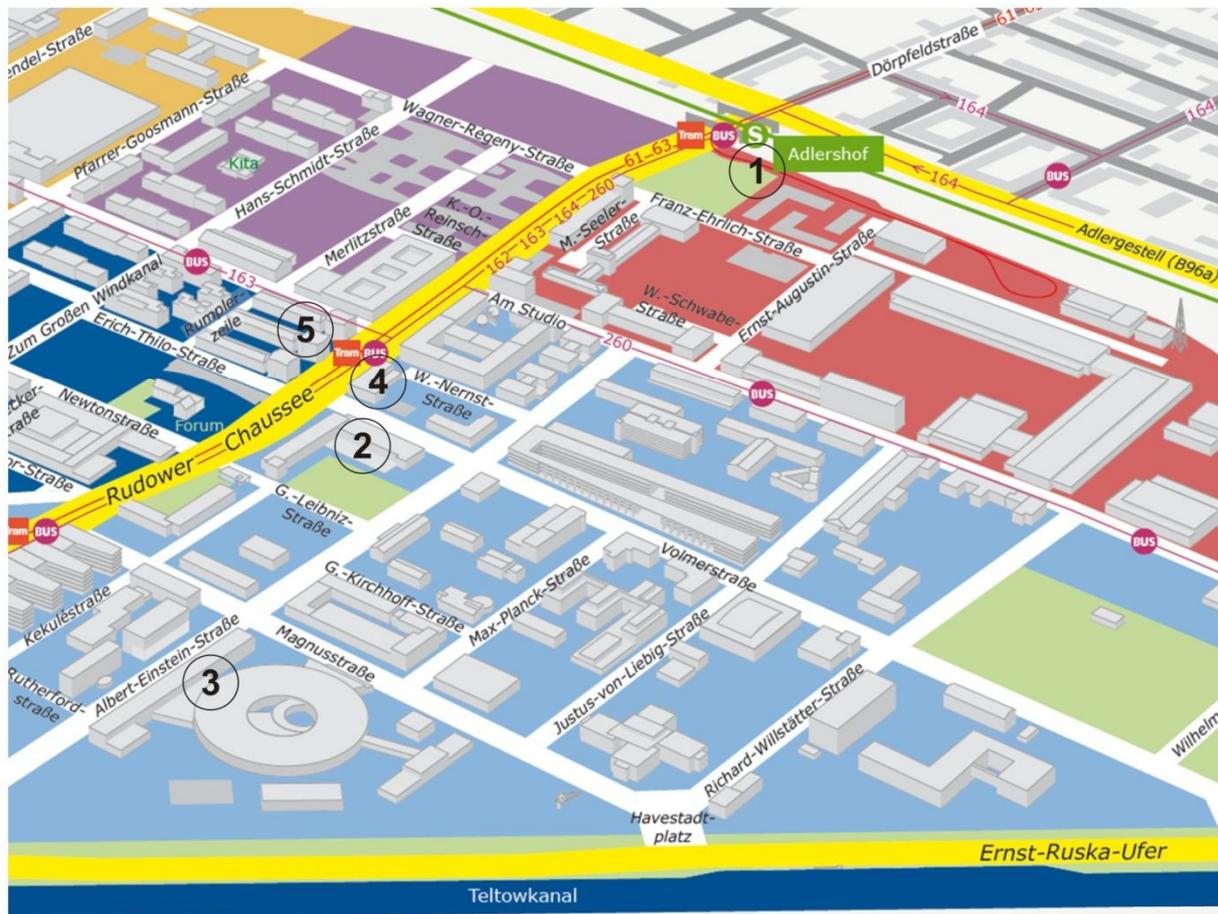
## Programme

Monday, 10. Oct. (Registration WISTA Centre)			
Welcome	Bernd Rech		9:00
<b>Overview Talks (Bunsen Saal, WISTA)</b>			<b>9:15-12:30</b>
Global Energy Challenge	Neal Armstrong	University of Arizona, USA	9:15
Solar Fuels	Roel van de Krol	HZB, DE	9:45
Photovoltaics	Christoph Brabec	Universität Erlangen, FAU, DE	10:15
Coffee (WISTA Centre)			10:45-11:15
Energy Storage	Andreas Züttel	EPFL, CH	11:15
Efficient Use of Energy	Emil List-Kratochvil	Humboldt Universität zu Berlin, DE	11:45
Welcome Address	Anke Kaysser-Pyzalla	HZB, DE	12:15
Lunch (WISTA Centre)			12:30-13:30
<b>Topical Sessions (Bunsen Saal, WISTA)</b>			<b>13:30-18:30</b>
Photovoltaics			
David Cahen	Weizmann Institute of Science, IL		13:30
Norbert Koch	Humboldt Universität zu Berlin, DE		14:00
Wim Sinke	University of Amsterdam, NL		14:30
Eva Unger	University of Lund, SE		15:00
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment			15:30
Coffee (WISTA Centre)			15:45-16:15
From Research to Products			
Martin Hermle	Fraunhofer ISE, DE		16:15
Stefan Koller	VARTA Micro Innovation, AT		16:45
Antonio Facchetti	Polyera, USA		17:15
Rutger Schlatmann	PVcomB, DE		17:45
Ideas, Suggestions and Requirements concerning industrial research at BESSY II			18:15
<b>End of the Day</b>			<b>18:30</b>

<b>Tuesday, 11. Oct. (Registration BESSY II Foyer)</b>		
Coffee (BESSY II Foyer)		8:30-9:00
<b>Topical Sessions (BESSY II Lecture hall)</b>		<b>9:00-11:15</b>
Solar Fuels and Catalysis		
Peter Strasser	Technische Universität Berlin, DE	09:00
Petra de Jongh	University of Utrecht, NL	09:30
Fraser Armstrong	University of Oxford, UK	10:00
Peter Wasserscheid	Universität Erlangen, FAU, DE	10:30
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		11:00
Lunch and Poster Session (BESSY II Foyer)		11:15-12:45
<b>Topical Sessions (BESSY II Lecture hall)</b>		<b>12:45-16:35</b>
Energy Storage and Batteries		
Jürgen Janek	Justus Liebig Universität Gießen, DE	12:45
Daniil Itkis	Lomonosov Moscow State University, RU	13:15
Frank Renner	Hasselt University, BE	13:45
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		14:15
Coffee (BESSY II Foyer)		14:25-14:55
Efficient Use of Energy		
Heiner Linke	Lund University, SE	14:55
Uli Lemmer	KIT, DE	15:25
Andy Thomas	IFW Dresden, DE	15:55
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		16:25
<b>Into the Future (BESSY II Lecture hall)</b>		<b>16:35-17:30</b>
Marcus Bär, SISSY@EMIL	HZB, DE	16:35
Axel Knop-Gericke, Cat@EMIL	FHI, MPG, DE	16:50
Roel van de Krol, HEMF	HZB, DE	17:05
General Discussion and Summary		17:20
<b>End of the Workshop / Visit of BESSY II</b>		<b>17:30</b>

## Site plan

### Helmholtz-Zentrum Berlin Wilhelm-Conrad-Röntgen Campus Adlershof



- ① Train Station Adlershof
- ② WISTA Centre: Registration 10th of October
- ③ HZB, BESSY II: Registration 11th of October

- Hotels:
- ④ Dorint
  - ⑤ Airport Hotel

Poster Session

**HZB, BESSY II**  
Albert-Einstein-Str. 15  
12489 Berlin

tel +49 (0)30 8062 - 12931  
fax +49 (0)30 8062 - 14746  
photons@helmholtz-berlin.de

## **Abstracts of the Overview Talks**

Monday, 10<sup>th</sup> of October

Location: WISTA Centre, Bunsen Saal

## Global Energy Challenges: The Energy/Water/Food Nexus

Neal R. Armstrong<sup>1,2</sup>

1 Department of Chemistry/Biochemistry , University of Arizona Tucson, Arizona USA

2 College of Optical Sciences Office for Research and Discovery, University of Arizona Tucson, Arizona USA

This talk will focus on some of the challenges we currently face in the efficient creation and use of energy and the link between energy and production of secure and sustainable sources of water and food, one of the most significant challenges of the 21<sup>st</sup> Century. We'll discuss these challenges, and the opportunities they present, in the context of the way life is changing in the western U.S. We recognize, however, that these problems and their solutions are common to many areas of the world currently experiencing "stress" to their supplies of clean water and food, while often being awash in underutilized and underappreciated supplies of renewable energy. The source of much of this overview comes from recent National Science Foundation and U.S. Department of Energy initiated workshops (the one held in Arizona can be found at: <http://energywaterfoodnexus.wordpress.com/>). Among the five themes that have emerged from these workshops (Situational Scarcity, New Materials and Technologies, Smart Data, Policy Responses and Test Beds) we see a need for development and integration of technology (demonstrated at scale), policy responses and public acceptance. Especially for the energy materials research communities we need to engage the end users of our new technologies at the earliest stages of research and development, and I will cite a few specific examples where energy conversion and energy storage, water purification and reuse, and food production may one day be integrated in ways that lead to more resilient communities.

## From Sunlight To Chemical Fuels

Roel van de Krol<sup>1,2</sup>

1 Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,  
Germany

2 Institut für Chemie, Technische Universität Berlin, Germany

The conversion of sunlight into chemical fuels is an elegant approach to address the need for long-term storage of solar energy. Using water and CO<sub>2</sub> as cheap and abundant resources, a wide variety of products can be obtained, ranging from hydrogen to liquid hydrocarbons. The first and arguably most important step in any of these processes is the splitting of water into hydrogen and oxygen. Several photoelectrochemical (PEC) routes for water splitting will be discussed. These range from state-of-the-art III-V semiconductors functionalized with noble metal catalysts to low-cost metal oxide powders dispersed in water. The challenge is to find semiconductors and catalysts that are stable, efficient, and affordable. Much progress has been made in the past 5 years, and the number of autonomous PEC water splitting with efficiencies >5% has rapidly grown. I will show some of the highlights and innovative approaches that have been developed, and discuss the key remaining challenges. Finally, I will briefly touch on some challenges in device engineering that need to be tackled Solar before PEC technology can become a reality.

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## **Solution Processed Semiconductors: Challenges and Opportunities of a Next Generation Photovoltaic Technology**

Christoph J. Brabec <sup>1,2</sup>

1 Friedrich Alexander University Erlangen-Nürnberg, Material Science, i-MEET,  
Martensstrasse 7, 91058 Erlangen, Germany

2 ZAE Bayern, Renewable Energies, Haberstrasse 2a, 91058 Erlangen, Germany

Solution processed semiconductors play an essential role in the future renewable energy scenarios where power generation by photovoltaics will be one of the pillars for the world's clean energy supply. The printed photovoltaics technology has evolved from purely organic to inorganic and most recently to hybrid semiconductor systems, being accompanied with an increase in efficiency from the 1 % regime in the 90s to the 20 % regime nowadays.

This presentation will outline the challenges for organic vs. perovskite based photovoltaic systems with a strong focus on the structure - property relations allowing to carefully keep the balance between stable and efficient microstructures.

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## From Renewable Energy to Synthetic Hydrocarbons

Andreas Züttel, Mariana Spodaryk, Noris Gallandat

1 LMER, ISIC, SB, École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis,  
Rue de l'Industrie 17, CP 440, CH-1951 Sion, Switzerland

2 Empa Material Science and Technology, Switzerland

Storage of renewable energy becomes more important with increasing contribution of renewable energy to the energy demand. Energy storage for mobility and seasonal storage are the two major challenges, because of the high energy density required and the large amount of stored energy. The technical solution is to produce hydrogen from renewable electricity and use the hydrogen to reduce CO<sub>2</sub> from the atmosphere in order to synthesize liquid hydrocarbons as energy carriers. This requires large scale electrolyzers, hydrogen storage, adsorption of CO<sub>2</sub> and finally a well controlled reaction of H<sub>2</sub> and CO<sub>2</sub> to a specific product, e.g. octane. The storage of liquid hydrocarbons is a well-established technology. The challenges and the solutions for the realization of the technical process have been analyzed in detail and a small scale demonstrator, the size corresponds to the world average energy consumption per capita, has been built.

The objectives of the demonstrator are to investigate the energy flow from renewable source to hydrocarbons under real conditions; to build a database of energy flows and energy storage for the system modeling; to build a platform for testing new components with new materials and to demonstrate a working conversion from solar energy to hydrogen and hydrocarbons with a size corresponding to average global energy consumption per capita; to compare components e.g. different types of photovoltaic cells, different batteries under working conditions and to create an economic database of the components and investigate the lifetime; to stimulate the collaboration between the research groups in Energypolis and to develop new products and create startup companies; to stimulate the collaboration with academic partners worldwide and to create a platform for services, research and development with industry.

## **Efficient Use of Energy: Additive Manufacturing of Light Emitting Devices**

Emil J.W. List-Kratochvil

Humboldt-Universität zu Berlin, Institut für Physik, Institut für Chemie & IRIS  
Adlershof, Brook-Taylor-Straße 6, 12489 Berlin, Germany

More than 20% of the world's total electricity consumption is used for lighting applications and an estimate of 25% when including display and TV applications. Therefore, innovative, cost and energy efficient solutions for lighting and display applications are in the focus of an ongoing intense worldwide and European effort in the field of photonics research and development. In particular, light emitting organic light emitting diodes (OLED) as well as inorganic solid state lighting technologies are the most promising candidates for the lighting revolution of the 21<sup>st</sup> century with the potential to save hundreds of GWh or millions tons of coal/year if put in place. Yet, despite first promising commercial success of the OLED technology, a number of challenges need to be further addressed to allow full exploitation of its potential. Along with the ever ongoing quest for emitter materials with improved stability and reliable structure to property relations, in particular cost- and energy efficient low temperature production through printing techniques need to be addressed. Among different available coating and printing techniques 2D and 3D inkjet printing (IJP) has become popular as a flexible (digital), additive, selective and cost- and energy-efficient material deposition method for electronic and photonic materials. The main emphasis of this talk will be to highlight on how scientific knowledge gained in material and device research may turn into industrial relevant processes, applications and product development based on OLEDs.

## **Abstracts of the Photovoltaics Session**

Monday, 10<sup>th</sup> of October

Location: WISTA Centre, Bunsen Saal

## Halide Perovskites, how special are they?

David Cahen

Materials & Interfaces Dept., Weizmann Inst. of Science, Rehovot, Israel 76100

Rather than what was and is often said, thought and written, halide perovskites are, with the notable exceptions of their elastomechanics, defect chemistry and physics, quite normal inorganic semiconductors. Thus, and care should be taken in comparing them with organic semiconductors and to describe their PV or LED behaviour with concepts from OPV, OLEDs and dye-sensitized solar cells. Still, there are the above-stated exceptions that allow making excellent quality optoelectronic materials in a very fast, low temperature process, from solution. **This is amazing for electronic materials research.** To make progress to understand this behavior, we look for, and scrutinize apparent inconsistencies in these materials, such as high carrier lifetimes *cum* modest mobilities, low temperature preparation *cum* low defect density, apparently flexible inorganic lattice *cum* very sharp diffraction and sharp optical absorption onsets. I will discuss progress towards understanding these issues.

## **Energy materials research with photoemission spectroscopy: Challenges and opportunities**

Norbert Koch<sup>1,2</sup>

1 Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

2 Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Research on modern and emerging energy materials relies on a robust and reliable understanding of the materials' electronic structure. This prerequisite enables developing methods for optimizing material processing and heterojunction formation in terms of reaching true electronic grade, which is indispensable for applications. Traditionally, photoemission spectroscopy (PES) is a primary instrumental methods to determine the electronic structure. By using synchrotron radiation the method gains substantial impetus as the photon energy can be selected from the UV- to the hard X-ray regime. One drawback of PES, however, is that it is notoriously difficult to obtain reliable data for materials that are poorly conductive (resulting in sample surface charging) or radiation sensitive (resulting in defect state creation). Many energy materials currently attracting huge interest fall into this class, e.g., metal oxides, perovskites, and organic semiconductors. One obvious solution to the problem is suitably reducing the photon flux, which comes at the cost of lower photoelectron count rates. Examples for these challenges and how they can be resolved, also by employing more efficient electron analyzers, will be discussed for emerging materials of interest for photovoltaics and light emitting diodes, i.e., perovskites and organic semiconductors.

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## Photovoltaics to and beyond ultra-low-cost electricity

Wim C. Sinke<sup>1,2,3</sup>

1 ECN Solar Energy, The Netherlands

2 University of Amsterdam and FOM Institute AMOLF, The Netherlands

3 European Technology and Innovation Platform for Photovoltaics (ETIP PV)

Photovoltaic solar energy (PV) is a key technology for the transformation of our energy system, leading to very low carbon emissions and security of supply and contributing to a new, green (or blue) economy. In combination with other renewables and energy storage, it will enable a sustainable, affordable and reliable energy supply. PV has made impressive progress in terms of conversion efficiency, cost and scale of deployment. Power Purchasing Agreement (PPA) offers as low as 0.03 US\$/kWh in sunny regions have been announced recently. Further developments and breakthroughs in science, technology, system design and engineering, operation and maintenance, and a range of other aspects may well bring down costs by another factor of 3, leading to ultra-low Levelized Cost of Electricity (LCoE) around 0.01 US\$/kWh in high-insolation regions (and in the range of 0.02 to 0.03 US\$/kWh in moderate climates), making generation costs no longer a limiting factor for large-scale deployment. At such low values, PV may also be used for competitive generation of low-temperature as well as high-temperature heat and possibly even (solar) fuels. This will help PV to reach high penetration levels, but will also help other sectors than the power sector only to become more sustainable.

This presentation will provide an overview of the state-of-the-art in PV technology and applications, some key factors to be addressed by research and other parts of the PV sector to achieve a further cost reduction, and a vision on what ultra-low-cost PV can do to help building a sustainable energy system.

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## Hybrid organic-inorganic semiconductors to boost commercial PV technology

Eva Unger<sup>1,2</sup>, David Sörell<sup>1</sup>, Lukas Kegelmann<sup>2</sup>, Steve Albrecht<sup>2</sup>, Klaus Jäger<sup>2</sup>, Bernd Rech<sup>2</sup>

1 Chemical Physics, Dep. of Chemistry, Lund University, Lund, Sweden

2 Inst. Silicon Photovoltaics, Helmholtz-Zentrum for Materials and Energy, Berlin, Germany

Hybrid organic-inorganic perovskites (HOIPs) are intriguing materials to develop hybrid tandem photovoltaic device technology. The ideal bandgap of HOIPs for monolithically integrated HOIP/Si tandem solar cells is 1.73 eV, which can be obtained by halide substitution in  $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ , equal to an approximate composition of  $x = 0.2$ . Mixed anion higher bandgap HOIPs exhibit photoinstability visible in phase segregation caused by ion redistribution in the material.

Heat and light have apparently opposing effects on mixed halide  $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$  perovskites. Heat homogenizes the halide distribution while light can induce in-homogenization due to bromide and iodide migrating and forming domains within the samples. This is often observed as dynamic changes to the photoluminescence spectra with the evolution of a low energy phase. Photoinstability and ion migration effects in mixed halide HOIPs correlate with the intrinsic disorder of the material.

Photochemical instabilities and the formation of lower energy states, limit the quasi-Fermi level splitting and hence define the maximum open circuit voltage in devices utilizing these materials. The intrinsic defect state density and non-radiative recombination cause performance losses in the absorber. On the device level, architecture as well as absorber layer coverage and selective contacts determine the overall performance. To navigate all possible obstacles in the demanding task of optimizing hybrid tandem HOIP devices for tandem applications, we need to distinguish between the different possible limiting factor and hopefully overcome some of them by either engineering better materials or more suitable device architectures.

## **Abstracts of the from Research to Products Session**

Monday, 10<sup>th</sup> of October

Location: WISTA Centre, Bunsen Saal

## Silicon Solar Cells – Current Production and Future Concepts

Martin Hermle<sup>1</sup>, Stefan W. Glunz<sup>1,2</sup>

1 Fraunhofer ISE, Germany

2 University of Freiburg, Germany

Silicon solar cells dominate PV market since decades. The cost reduction of the wafer cell and module production leads to levelized cost of electricity (LCOE) in Germany below 8 €ct. One strategy to further decrease the LCOE, is to increase the cell efficiency without substantially increasing the manufacturing costs. The PERC Concept (Passivated Emitter and Rear Contact) which is currently rolled out in production has led to an efficiency boost to record efficiencies above 22 % on industrial size areas. Incremental improvements which can further increase the efficiency will be shown and the limitations of the technologies will be discussed. Furthermore, alternative concepts and concepts beyond the state of the art will be presented which shows that silicon solar cells still have a bright future.

## **Silicon as Active Material for Lithium Ion Batteries – State of the Art or Distant Future**

S. Koller

VARTA Micro Innovation GmbH, Austria

Since the large automotive companies go ahead with the electrification of the power train, also the demand for more powerful electrochemical energy storage systems is growing. However not only the automotive industry requires more powerful accumulators. In the area of mobile consumer electronics, the proceedings of the last years are compensated by the rising energy demand of the devices. Accordingly, the doubling of the energy density of lithium ion batteries, since they were commercialized by Sony in 1991, increased only imperceptibly the operating time.

The specific energy of a lithium ion battery is given by the product of specific charge - more precisely the lithium storage ability per mass and the voltage difference of negative and positive electrode. As far as the negative electrode is concerned lithium and lithium compounds already represent the most reductive species of the electrochemical series. However carbonaceous materials that are used in state of the art lithium ion batteries are only able to store up to 1 lithium ion per 6 carbon atoms in the case of fully crystalline graphite, which results in a quite low specific charge of  $372 \text{ Ah}\cdot\text{kg}^{-1}$ . The application of metals or semi metalloids, which are able to store lithium under formation of an intermetallic phase represents a very promising alternative, whereat especially silicon has turned out as a very promising material. Within this talk advantages and disadvantages of different silicon based active material concepts in combination with the achievable energy density enhancement will be discussed.

## **Synthesis and Structural Characterization of Opto-Electronic Materials for Unconventional Electronics**

Antonio Facchetti

Department of Chemistry, Northwestern University and Polyera Corporation, 2145 Sheridan Road, Evanston IL 60208, USA

a-facchetti@northwestern.edu

Printed electronics is a new technology envisioning the fabrication of electronic devices using solution processable materials and printing methodologies. In this presentation I will describe the materials synthesis, development, and process engineering enabling the fabrication of unconventional electronic and opto-electronic devices, such as transistors, circuits and solar modules, all on flexible foils using several new materials. Materials development include new synthetic, green routes to semiconducting polymers. Examples of unconventional electronic materials include organic small molecular and polymeric semiconductors, metal chelates and complexes, and hybrid organic-inorganic metal oxides. Materials structural characterization include single crystal XRD, specular XRD, GIWAX, XPS, TEM, AFM, and PAS to cite just a few examples. Thus, we will show the fabrication of polymer based complementary circuits with excellent performance (field-effect mobilities  $\sim 1\text{-}6\text{ cm}^2/\text{Vs}$ ), flexible amorphous oxides TFTs (field-effect mobilities  $\sim 5\text{-}40\text{ cm}^2/\text{Vs}$ ), polymeric donor-fullerene solar cells with efficiencies approaching 11% in inverted architectures, and new printed sensors with excellent sensitivity and detectivity.

## **Transferring thin film technology into photovoltaic applications**

Rutger Schlatmann<sup>1,2</sup>

1 Helmholtz Zentrum Berlin / PVcomB

2 Hochschule für Technik und Wirtschaft Berlin (HTW)

In this presentation, we will discuss the challenges connected to transfer of thin film technology into photovoltaic applications. We will discuss the requirements on PV materials and device structures for future applications. Next to functional demands, the cost of materials and equipment plays a crucial role for this mass application.

Specifically, we will highlight some examples of the direct connection between synchrotron based research and the development of next generation materials and equipment.

## **Abstracts of the Solar Fuels and Catalysis Session**

Tuesday, 11<sup>th</sup> of October

Location: BESSY II Lecture hall

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## Electrochemical Energy Materials: up-close and personal

Peter Strasser

Department of Chemistry, Chemical Engineering Division, Technical University Berlin,  
Germany

Catalysts are key electrode components of electrochemical galvanic and electrolytic energy cells used for storing and converting electricity. Their successful development and optimization requires time-, electrode potential-, and space-resolved insight into the atomic-scale chemical structure of the electrified interface and its correlation with catalytic activity, selectivity, and stability. This intimate insight critically depends on the availability of ex-situ, in-situ, or better operando analysis techniques suitable for the solid-liquid interface.

In this presentation I will highlight some recent studies [1-8] where photon- and electron- based characterization methods have advanced our knowledge and understanding of the active geometric and electronic structure of electrocatalytic energy nanomaterials during catalytic operation inside electrochemical energy cells. Examples will include Pt- and Pt alloy based nanomaterials for fuel cells, Ir-based oxide catalysts for acid electrolyzers, as well as non-precious transition metal oxide catalysts for solar fuel reactors.

### References:

- [1] Bergmann, A., E. Martinez-Moreno, D. Teschner, P. Chernev, M. Gliech, J. F. de Araujo, T. Reier, H. Dau and P. Strasser (2015) *Nature Communications* 6:8625
- [2] Goerlin, M., P. Chernev, J. F. De Araujo, T. Reier, S. Dresp, B. Paul, R. Kraehnert, H. Dau and P. Strasser (2016). *J. Am. Chem. Soc.* 138: 5603-5614.
- [3] Reier, T., Z. Pawolek, S. Cherevko, M. Bruns, T. Jones, D. Teschner, S. Selve, A. Bergmann, H. N. Nong, R. Schlögl, K. J. J. Mayrhofer and P. Strasser (2015) *J. Am. Chem. Soc.* 137: 13031- 13040.
- [4] Mistry, H., A. S. Varela, S. Kühl, P. Strasser and B. R. Cuenya (2016) *Nature Reviews Materials*: 16009.
- [5] Sahraie, N. R., U. I. Kramm, J. Steinberg, Y. J. Zhang, A. Thomas, T. Reier, J. P. Paraknowitsch and P. Strasser (2015). *Nature Communications* 6:8618.
- [6] Varela, A. S., N. Ranjbar Sahraie, J. Steinberg, W. Ju, H.-S. Oh and P. Strasser (2015). *Angewandte Chemie International Edition* 54: 10758-10762.
- [7] Vera Beermann, M. G., Elena Willinger, Stefan Rudi, Marc Heggen, Rafal E. Dunin-Borkowski, Marc-Georg Willinger, and Peter Strasser (2016). *Nano Lett.* 16: 1719–1725.
- [8] Gan, L., C. Cui, M. Heggen, F. Dionigi, S. Rudi and P. Strasser (2014). *Science* 346(6216): 1502-1506.

## Particle Size Effects in Catalysis

Petra E. de Jongh

Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Universiteitsweg 99, 3584 CG Utrecht, The Netherlands

[P.E.deJongh@uu.nl](mailto:P.E.deJongh@uu.nl)

Catalysts typically consist of supported metal particles. As the catalytic activity is associated with the surface of the metal particles, in general small metal particles are used, to optimize the specific metal surface area. Interestingly this does not always mean that the smaller the metal particle size is, the better. An interesting example is for instance the in-depth study of the Co particle size effect in Fischer Tropsch synthesis, where a very sharp optimum is found at 6-8 nm particle size.<sup>1</sup> In the vast majority of cases an optimum is found, although the exact reason is seldomly understood. This is partially due to the fact that it is generally a great challenge to change *only* the metal particle size without changing several other properties of the catalyst (such as pore size, loading, or support structure) at the same time.

A key tool to study particle size effects in our group is to first obtain a fundamental insight into the preparation pathway.<sup>2,3</sup> Model supports, such as carbon nanofibres or ordered porous oxides, can help to study the pure particle size effects. A second important tool is being able to investigate the performance of these catalysts (activity, selectivity and stability) under conditions as closely as possible mimicking industrial process conditions in terms of temperature, pressure and conversion. I will as a first example discuss the particle size effects, most notable on activity and selectivity, of supported Ag catalysts for ethylene epoxidation. In a second example I will go into more detail regarding recent results for supported Cu catalysts for methanol synthesis.<sup>4</sup>

### References:

- [1] J. Am. Chem. Soc. 128, 3956 (2006)
- [2] Chem. Rev. 115, 6687 (2015)
- [3] Appl. Catal. B 192, 199 (2016);
- [4] Nature Comm. DOI 10.1038/ncomms13057 (2016)

## Electrocatalysis for Energy – Learning from Enzymes

Fraser A. Armstrong

Department of Chemistry, University of Oxford

Despite their giant nature, enzymes are remarkable electrocatalysts. Attached to a suitable electrode, many enzymes catalyse reactions of great importance with rates and efficiencies that far outperform the catalysts being developed by chemists. Hydrogenases, which contain iron or iron and nickel, operate reversibly like platinum - they catalyse hydrogen production and hydrogen oxidation with minimal overpotential requirement. Likewise, some CO<sub>2</sub> reducing enzymes, also based on abundant elements, operate close to the reversible limit. How can we benefit from this knowledge? Direct use of enzymes as electrocatalysts is limited to those producing chemicals with high commercial value, thus ruling out any role in fuel production, but we can still learn some important lessons. This lecture will examine ways in which the remarkable electrocatalytic properties of enzymes are measured, mimicked and exploited.

Reference:

Reversibility and Efficiency in Electrocatalytic Energy Conversion and Lessons from Enzymes. F. A. Armstrong and J. Hirst. Proc. Natl. Acad. Sci. USA 108, 14049 (2011).

## Chemical Energy Storage

Peter Wasserscheid<sup>1,2</sup>

1 Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen, Germany

2 Forschungszentrum Jülich, „Helmholtz-Institut Erlangen-Nürnberg“ (IEK-11), Nögelsbachstrasse 49b, 91052 Erlangen, Germany

[peter.wasserscheid@fau.de](mailto:peter.wasserscheid@fau.de)

Hydrogen is often considered a very capable future energy vector as it can be produced from wind or solar power via water electrolysis and finds use in various energy applications. The gravimetric energy storage density of hydrogen is excellent (33.3 kWhkg<sup>-1</sup> (LHV)). However, its volumetric storage density is only 3 Wh/liter at ambient pressure. In existing technical applications hydrogen is therefore either stored under very high pressures (up to 700 bar) or in its liquid state at 253 °C to reach acceptable storage densities.

A very attractive way to store and release hydrogen is in form of “Liquid Organic Hydrogen Carriers” (LOHC) systems [1]. Aromatic molecules, such as dibenzyltoluenes [2], can be reversibly hydrogenated and dehydrogenated in order to store and transport large amounts of hydrogen in form of diesel-like liquids. The presentation introduces shortly the LOHC concept and compares it to other methods of chemical energy storage. Afterwards, mechanistic and reaction engineering aspects of the catalytic LOHC hydrogenation and dehydrogenation processes are discussed. On-going surface science studies [3] and kinetic investigations are described [4]. Applications and future application scenarios of the technology will be presented.

### References:

- [1] D. Teichmann, W. Arlt, P. Wasserscheid, R. Freymann, *Energy Environ. Sci.* 4(8), 2767-2773 (2011).
- [2] N. Brückner, K. Obesser, A. Bösmann, D. Teichmann, W. Arlt, J. Dungs, P. Wasserscheid, *ChemSusChem* 7(1), 229-235 (2014).
- [3] C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, *Chemical Record* 14(5), 879-896 (2014).
- [4] W. Peters, A. Seidel, S. Herzog, A. Bösmann, W. Schwieger, P. Wasserscheid, *Energy & Environmental Science*, 2015, 8, 3013-3021.

## **Abstracts of the Energy Storage and Batteries Session**

Tuesday, 11<sup>th</sup> of October

Location: BESSY II Lecture hall

## “Next generation” batteries and underlying cell reactions

Jürgen Janek<sup>1,2</sup>, Daniel Schröder<sup>1</sup>, Wolfgang Zeier<sup>1</sup> and Joachim Sann<sup>1</sup>

1 Institute of Physical Chemistry & Laboratory of Materials Science, Justus Liebig University, Gießen, Germany

2 BELLA, Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

The electrochemical characterization of batteries offers detailed phenomenological information, but does not provide unequivocal chemical information. Thus, true mechanistic information on electrochemical reactions can only be gained by coupling electrochemical measurements to spectroscopic, spectrometric, diffraction/scattering or microscopic techniques. In this lecture an overview on different types of next-generation battery systems and their cell reactions is given, and the role of spectroscopic in situ and operando techniques along with in situ diffraction is highlighted. Important examples will be metal-air, alkali metal-sulfur and solid state batteries. The role of synchrotron based methods is emphasized, as laboratory-scale techniques often do not offer enough sensitivity.

### References:

- [1] *In operando x-ray tomography for next-generation batteries: A systematic approach to monitor reaction product distribution and transport processes*, D. Schröder, C. L. Bender, T. Arlt, M. Osenberg, A. Hilger, S. Risse, M. Ballauff, J. Janek, I. Manke, *J. Phys. D: Appl. Phys.* **49** (2016) 404001
- [2] *Insights into the chemical nature and formation mechanisms of discharge products in Na-O<sub>2</sub> batteries by means of operando X-ray diffraction*, R. Pinedo, D. Weber, B. Bergner, P. Adelhelm, and J. Janek, *J. Phys. Chem. C* **120** (2016) 8472-8481
- [3] *Visualizing Current-Dependent Morphology and Distribution of Discharge Products in Sodium-Oxygen Battery Cathodes*, D. Schröder, C. L. Bender, M. Osenberg, A. Hilger, I. Manke, and J. Janek, *Sci. Rep.* **6** (2016) 24288

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## Challenges Facing the Development of Electrode Materials for Lithium-Air Batteries

D.M. Itkis<sup>1</sup>, E.Yu. Kataev<sup>1</sup>, A.I. Belova<sup>1</sup>, A.Ya. Kozmenkova<sup>1</sup>, T.K. Zakharchenko<sup>1</sup>, A.A. Rulev<sup>1</sup>, O.O. Kapitanova<sup>1</sup>, J.J. Velasco-Velez<sup>2</sup>, A. Knop-Gericke<sup>2</sup>, L. Gregoratti<sup>3</sup>, M. Amatti<sup>3</sup>, D.V. Vyalikh<sup>4</sup>, V. Perez-Dieste<sup>5</sup>, C. Escudero<sup>5</sup>, M.V. Avdeev<sup>6</sup>, V.I. Petrenko<sup>6</sup>, D.G. Kwabi<sup>7</sup>, H.H. Chang<sup>7</sup>, Y. Shao-Horn<sup>7</sup>, L.V. Yashina<sup>1</sup>

1 Lomonosov Moscow State University, Russia

2 Fritz Haber Institute, Germany

3 ELETTRA Sincrotrone Trieste, Italy

4 Donostia International Physics Center, Spain

5 ALBA Synchrotron, Spain

6 Joint Institute for Nuclear Research, Russia

7 Massachusetts Institute of Technology, USA

Lithium-oxygen chemistry can potentially enable development of rechargeable batteries demonstrating a few-fold increased specific energy in comparison to lithium-ion ones. The practical implementation of this idea, however, faces a number of significant challenges. The first one is the problem of positive electrode material stability during cycling. During lithium-air battery (LAB) operation oxygen reduction reaction occurs at the positive electrode – oxygen dissolved in the electrolyte is reduced to superoxide ( $O_2^-$ ), which forms ionic pairs with  $Li^+$  ( $LiO_2$ ). Such intermediates are then converted to a final discharge product lithium peroxide ( $Li_2O_2$ ) after transfer of second electron from the electrode or by chemical disproportionation reaction. Unfortunately, oxygen reduction products and intermediates are highly reactive species that can attack both electrolyte solvents and electrode materials. Among others, carbon materials received major attention as a positive electrode in  $Li-O_2$  cells as they are freely available, porous, highly conductive and lightweight. The requirements for porous positive electrodes and their chemical stability would be discussed in the talk using carbon materials and Ti-based conductive compounds as an examples. Issues connected with negative electrode, namely SEI formation on metallic lithium electrodes and dendrite growth would be also considered. Application of a number of neutron and synchrotron-based tools (SANS, neutron reflectometry, XPS/NAP XPS and others) for monitoring the interfacial processes at both negative and positive electrodes will be demonstrated.

## Combining complementary techniques: How Hard X-Ray Photoelectron Spectroscopy can help to control the SEI on silicon

Frank Uwe Renner<sup>1,2</sup>

1 Hasselt University, Institute for Materials Research IMO, Diepenbeek, Belgium

2 IMEC vzw. Division IMOMECE, Wetenschapspark 1, Diepenbeek, Belgium

The combination of organic electrolytes, reactive Li metal, and ions, and of alloying and intercalation reactions with associated volume changes render Li-ion batteries (LIBs) complex electrochemical systems. A potential development of a new Li-ion battery system needs to fulfill severe requirements, among others progress in specific capacity and energy density as well as in cycle life, reliability and safety. Future lithium-ion batteries are considered for a broad range of applications beyond the initial use in consumer electronics, from electric vehicles (EV) to off-grid or home energy storage for example in combination with photovoltaic systems. Advanced characterization techniques can help the development and allow deep insights in acting mechanisms – preferably at the atomic or low-nanometer scale and performed in-situ<sup>1,2</sup>. As a matter of fact electrochemical interfaces are controlled by (applied) potentials and may significantly change at open circuit conditions. They are also buried in electrolyte and may quickly react in contact with other media. These latter facts make electrochemical research both challenging and interesting at the same time. Techniques based on synchrotron light such as in-situ X-ray Diffraction (in-situ XRD) or Hard X-Ray Photoelectron Spectroscopy (HAXPES) can complement electrochemical testing for battery research, but also lab-based methods as for example Atom Probe Tomography (APT) or Surface Force Apparatus (SFA) measurements<sup>1</sup> offer unprecedented insights. I will describe recent applications of the latter techniques for our research on Si and Si-alloy interfaces and solid electrolyte interphase (SEI) formation. By using HAXPES the influence of the new formula of electrolytes has been investigated comparing the electrochemical performance and SEI formation between Si and Si-alloy half-cells cycled with modified electrolytes. Indications for improvements in capacity and retention were obtained using FEC as the major component in the electrolyte for Si alloys or using additives for pure Si active material. The conformal SEI layer on the alloy particles showed less decomposition product at lithiated stage, indicating a thinner and more homogeneous SEI generation.

### References:

[1] Moeremans et al., Dynamic Wetting Phenomena of Nano-Confined Graphene by Lithium-Ion Battery Electrolyte, *Nature Communications* 2016, 7, 12693.

[2] Bach et al., Structural changes during lithiation cycles of Li-Au observed by in-situ high-energy x-ray diffraction, *Chem. Mater.*, 2016, 28, 2941

## **Abstracts of the Efficient Use of Energy Session**

Tuesday, 11<sup>th</sup> of October

Location: BESSY II Lecture hall

## Hot-carrier solar cells: thermoelectrics to enhance photovoltaics

Heiner Linke

NanoLund and Solid State Physics, Lund University, Sweden

A fundamental limit to the performance of conventional photovoltaic devices is that photogenerated electrons and holes in semiconductors lose part of their energy via phonon emission, which ‘cools’ the carriers to the lattice temperature. It has been suggested that carrier energy filters could be used to separate high-energy (hot) electron-hole pairs before they cool, to thereby boost device performance, and to specifically increase the open-circuit voltage ( $V_{oc}$ ) by up to hundreds of millivolts. However, this has so far not been realized, primarily because sufficiently fast charge separation of hot, photogenerated electron-hole pairs is difficult to achieve in the planar devices used so far.

Here, we establish the conditions under which hot carrier solar cells can be operated reversibly, that is, at maximum energy conversion efficiency. We find that, under specific conditions, the energy conversion efficiency of a hot carrier solar cell can exceed the Carnot limit set by the intra-device temperature gradient alone, due to the additional contribution of the quasi-Fermi level splitting in the absorber [1]. Furthermore, we report first experiments in InAs/InP heterostructure nanowires, demonstrating an open circuit voltage that exceeds that achievable with traditional photovoltaic devices based on a single bandgap [2].

References:

[1] Limpert et al, New J. Phys 17 095004 (2015)

[2] Limpert et al., submitted (2016)

## Printed Energy Conversion Devices

U. Lemmer<sup>1,2,3</sup>

1 Light Technology Institute, Karlsruhe Institute of Technology (KIT), Germany

2 Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), Germany

3 InnovationLab, Speyerer Str. 4, Heidelberg

Solution processable (“printable”) materials such as conjugated polymers, semiconductor nanoparticles, oxide and metal precursors combine the ease of processing with interesting optical and electronic properties. The potential cost effective fabrication of large area devices based on solution processing has brought these materials into the focus of emerging photovoltaic, and light emitting technologies. More recently, these materials have also shown quite high efficiencies in thermoelectric generators. The presentation will give an overview over the different requirements for the functional layers in these energy conversion devices. The contribution will also cover recent progress in device architectures and corresponding printing and processing technologies. Even quite impressive efficiencies have been reached, many fundamental issues concerning a microscopic understanding of the transport properties are not well understood. This is particularly true for the large number of organic-organic and organic-inorganic internal interfaces.

### References:

S. Gärtner, S. Reich, M. Bruns, J. Czolk, A. Colsmann, *Nanoscale* 8, 6721, (2016)

S. Tekoglu, M. Petzoldt, S. Stolz, U. H. F. Bunz, U. Lemmer, M. Hamburger, G. Hernandez-Sosa, *ACS Appl. Mater. Interfaces* 8, 7320, (2016)

## Chalcogenide-type nanostructures: Interplay between Thermoelectric and Topological Insulators Properties

Andy Thomas, Kornelius Nielsch

Institute for Metallic Materials, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

We look into the connection between the thermoelectric performance and the characterizing features of topological insulators in chalcogenide-type materials. While topological surface states seem to play a minor role in the thermoelectric transport in bulk materials [1], it will be shown that they strongly contribute to the transport in nanostructures due to their high surface-to-volume ratio [2-4]. Specifically, thermoelectric and magnetotransport experiments on ALD-grown  $\text{Sb}_2\text{Te}_3$  thin films as well as on VLS-grown  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  nanowires are presented and the results are interpreted using thermoelectric transport calculations [5]. In all investigated systems, the maximum TE performance converges towards the maximum TE performance of the surface states with decreasing system size into the nanometer-range, limiting their application in efficient thermoelectric devices.

### References:

- [1] Kornelius Nielsch, Julien Bachmann, Johannes Kimling, and Harald Böttner, *Thermoelectric Nanostructures: From Physical Model Systems towards Nanograined Composites*, Adv. Eng. Mater. **1** (2011) 713-731.
- [2] Bacel Hamdou, Johannes Gooth, August Dorn, Eckhard Pippel, and Kornelius Nielsch, *Aharonov-Bohm oscillations and weak antilocalization in topological insulator  $\text{Sb}_2\text{Te}_3$  nanowires*, Appl. Phys. Lett. **102** (2013) 22110.
- [3] Bacel Hamdou, Johannes Gooth, August Dorn, Eckhard Pippel, and Kornelius Nielsch, *Surface state dominated transport in topological insulator  $\text{Bi}_2\text{Te}_3$  nanowires*, Appl. Phys. Lett. **103** (2013) 193107.
- [4] Johannes Gooth, Bacel Hamdou, August Dorn, Robert Zierold, and Kornelius Nielsch, *Resolving the Dirac cone on the surface of  $\text{Bi}_2\text{Te}_3$  topological insulator nanowires by field-effect measurements*, Appl. Phys. Lett. **104** (2014) 243115.
- [5] Johannes Gooth, Jan Goeran Glusckke, Robert Zierold, Martin Leijnse, Heiner Linke, Kornelius Nielsch, *Thermoelectric performance of classical topological insulator nanowires*, Semicond. Sci. Technol. **30** (2015) 015015.

## **Poster Abstracts**

Tuesday, 11<sup>th</sup> of October

Location: BESSY II Foyer

## **1 User Service for Energy Material Science Research**

Bettina Wolter, Britta Höpfner, Astrid Brandt, Florian Staier, Antje Vollmer

We intend to present the User Service at the Storage Ring BESSY II, the HZB CoreLabs, HEMF and Sample Environment at HZB.

## **2 High-activity catalyst films for water oxidation based on transition metal alloys**

Stefan Loos, Holger Dau

Oxy-hydroxide materials containing Fe and Ni have consistently been reported to exhibit electrocatalytic water oxidation performance that rivals that of conventional iridium oxide anodes. We report a simple, low-cost electrochemical approach to convert transition metal alloys into electrocatalysts with outstanding electrocatalytic water oxidation properties ( $<300 \text{ mV}@10 \text{ mA cm}^{-2}$ , Tafel slopes of  $30\text{-}40 \text{ mV decade}^{-1}$ ) and high stability in alkaline medium. EXAFS-analysis provides evidence of  $\mu_2$ -oxo bridged metal centers with octahedral coordinated oxygen ligands. In line with XPS-studies the oxidation states under open circuit conditions can be determined as +2 for nickel and +3 for the iron.

## **3 3D Direct Visualization of the Morphological and Chemical Changes in Plant Cell Wall Deconstruction**

Rodolfo Conti, Luciano A. Montoro, Felipe Antunes, Henning Markötter, André Hilger, Silvio Silvério da Silva, Ingo Manke, Augusta Isaac

Phase-contrast tomography (PCT) has emerged as a powerful tool for the three-dimensional characterization of plant tissue architecture. Here, PCT capabilities were extended to probe the 3D chemical distribution in bulk materials. Examining the plant tissue architecture in tandem with chemical distribution, new insights into the underlying mechanisms of pretreatments are provided. Sugarcane bagasse and sequential acid-base pretreatments were investigated to shed light on substrate-related features that limit sugar release.

## **4 Investigation of energy harvesting processes by soft X-ray photoelectron and absorption spectroscopies at solid-liquid interfaces**

Velasco-Velez J.J., Pfeifer V., Hävecker M., Skorupska K., Stotz E., Schlögl R., Knop-Gericke A.

One of the main goals in electrochemistry is the characterization of electrode-electrolyte interfaces under operating conditions [1]. The lack of surface sensitive techniques able to monitor the electronic structure under such conditions hinders the total understanding of such processes. We overcome this issue with a new setup based in a bi-layer graphene membrane making possible PES *in situ* [2]. Our method opens the way for studies of any solid-liquid or solid-gas [3] interfaces.

[1] Velasco-Velez, J. J. et al (2014), *Science*, 346(6211), 831-834. [2] Velasco-Velez, J. J. et al (2015), *Angewandte Chemie International Edition*, 54(48), 14554-14558. [3] Velasco-Vélez, J. J. et al (2016), *Review of Scientific Instruments*, 87(5), 053121.

## **5 Influence of annealing treatment on thermoelectric properties of MBE grown ZnO**

K. Mahmood, B.M. Samaa, M. Asghar

We report the influence of temperature and environment on thermoelectric properties of MBE grown ZnO on Si. A set of grown ZnO was annealed in O<sub>2</sub> and another set was annealed in different environments. Seebeck measurements showed that Seebeck coefficient and power factor increased with increasing temperature. XRD results demonstrated that FWHM of ZnO(002) decreased and crystalline size increased with increasing temperature. Photoluminescence study revealed that the intensity of band edge emission increased and defect emission decreased with increasing temperature because the density of O<sub>2</sub> vacancy related donor defects decreased with annealing temperature.

## **6 Characterisation of Nanostructures for Supercapacitors, Batteries and Solar Cells using advanced Synchrotron Scattering Techniques**

R.T. Lechner, C. Prehal, C. Koczwara, G. Fritz-Popovski, O. Paris

In this contribution we will show synchrotron in-operando studies on the behaviour of electrolyte ions in nanopores of supercapacitors [1] and on the structural changes of nanocrystals during cycling in Li-ion batteries. Furthermore, we will present ex-situ contrast variation studies to obtain the chemical and crystalline profile of PbS/CdS core/shell nanocrystals for solar cell applications [2].

[1] C. Prehal, D. Weingarth, E. Perre, R.T. Lechner, et al., *Energy Environ. Sci.* 8, (2015), [2] R.T. Lechner, G. Fritz-Popovski, M. Yarema, et al., *Chem. Mater.* 26, (2014)

## **7 In Operando Study of MnPi Modified BiVO<sub>4</sub> photoanodes by Soft X-ray Absorption Spectroscopy**

Lifei Xi, Fuxian Wang, Christoph Schwanke, Fatwa F. Abdi, Ronny Golnak, Sebastian Fiechter, Klaus Ellmer, Roel van de Krol, and Kathrin M. Lange

In this study, we demonstrated for the first time that the PEC performance of BiVO<sub>4</sub> photoanode can be improved by MnPi modification. We further investigated the electronic structure information of Mn L-edge X-ray absorption (XA) spectrum using in operando soft XAS. The Mn L-edge spectra under different potentials and light conditions are investigated. Using linear combination method, the information of different Mn species are revealed. We found that charge transfer in the MnPi and electrolyte interface is affected by band bending which relates to applied potential and built-in potential. The present work should benefit the potential applications of other OECs on photoanodes.

## **8 Iridium oxide, membranes and buffers for (photo)electrochemical water-splitting: What have we learned?**

Nella M. Vargas-Barbosa

Different aspects critical in the design and optimization of solar fuel cells are highlighted: (1) The role of surface ligands and intermediates of colloidal iridium oxide as co-catalyst for the OER on photoanodes is described; (2) A systematic study of the resistive losses in water-splitting cells that utilize commercial ion exchange membranes and buffered electrolytes is presented; (3) the benefits and challenges of incorporating bipolar membranes in solar water-splitting cells are discussed.

## **9 Numerical results using FDTD method to simulate the surface Plasmons for circular silver cylinder**

Otman Sofiane, Said Ouaskit

Using the two-dimensional finite-difference time-domain (2D-FDTD) method, with the perfectly matched layer (PML), we can simulate the surface Plasmons (SPs). In this context, we based on the idea of effective permittivity for the curved surface applied to the dispersive media, while the Z-transform method is applied to the Drude model. The numerical results obtained by 2D-FDTD for circular silver cylinder is given.

## **10 Energy storage research in the Giessen junior research groups**

Matthias Elm, Jürgen Janek, Daniel Schröder, Wolfgang Zeier

The group of Mathias Elm focuses on the electrical transport processes in purely ionic and mix ionic-electronic conducting microstructured and mesoporous ceramic oxides. The group of Daniel Schröder employs X-ray tomography and electrochemical studies to better understand metal-air batteries. The Zeier group focuses on structure-property relationships and design of functional materials for lithium ion conductors and all-solid state batteries.

## **11 X-ray Studies of Electrochemical Systems - Synchrotron Methods for Energy Materials**

Artur Braun

This poster presents a suite of operando and in situ studies on electrochemical energy materials, components and devices with x-ray and neutron methods.

## **12 Iron fluoride as cathode electroactive material for Li-Ion batteries**

L. Di Carlo, D. E. Conte, M. T. Sougrati, B. Fraisse, E. Kemnitz, L. Stievano, N. Pinna

The electrochemical reaction of HTB- $\text{FeF}_3 \cdot 0.33\text{H}_2\text{O}$  xerogel was studied by *operando* Mössbauer spectroscopy, evidencing the structural collapse of the HTB phase and the gradual and irreversible transformation into  $\text{FeF}_2$ -rutile-like nanodomains. Optimization of the material allowed the production of a nanostructured RGO-based composite, which was able to sustain repeated cycling at different C-rates and recovered full capacity after more than 50 cycles with respect to the unsupported  $\text{FeF}_3 \cdot 0.33\text{H}_2\text{O}$ .

### **13 In-situ investigations on the norbornadiene/quadricyclane energy storage system on various metal surfaces by UPS and high-resolution-XPS**

Udo Bauer, Philipp Bachmann, Florian Späth, Fabian Düll, Christian Papp, Hans-Peter Steinrück

Strained organic molecules, e.g. quadricyclane (QC) and its strain-released counterpart norbornadiene (NBD) are candidates for an energy storage system. By absorption of light, NBD is transformed to QC, followed by a catalytic energy release to reform NBD. We investigated the adsorption of QC and its conversion to NBD on Pt(111). UPS provides characteristic spectra of NBD/QC. We observe the conversion of QC to NBD below 120 K. HR-XPS reveals the decomposition of NBD at higher temperatures. The work was supported by the Cluster of Excellence Engineering of Advanced Materials (EAM).

### **14 $\text{Cu}_2\text{ZnGe}(\text{S},\text{Se})_4$ absorber formation studied by soft and hard x-ray photoelectron spectroscopy: Impact of precursor composition**

X. Kozina, T. Schnabel, T. Kunze, D. Gerlach, S. Ueda, R.G. Wilks, E. Ahlsweide, and M. Bär

In this contribution, we present a spectroscopic investigation of the processing steps for solution-deposited  $\text{Cu}_2\text{ZnGeSSe}_4$  (CZGSSe) thin films. The effect of different precursor composition, specifically different oxidation states of the Ge and Cu precursor on the chemical and electronic structure of the ultimately formed CZGSSe absorber film is investigated by soft (XPS) and hard (HAXPES) x-ray photoelectron spectroscopy at EMIL and at SPring-8.

### **15 Annealing-induced (optoelectronic) structure changes of $\text{In}_2\text{O}_3$ variants**

T. Xiao, H. Scherg-Kurmes, S. Körner, M. Meixner, X. Kozina, E. Ikenaga, R. Florian, R. Félix, X.X. Liao, R.G. Wilks, B. Szyszka, and M. Bär

$\text{In}_2\text{O}_3$  variants are prominent transparent conductive oxides that have widespread applications due to its high optical transparency and electrical conductivity. Films of intrinsic and Sn or H doped  $\text{In}_2\text{O}_3$  prepared by RF magnetron sputtering have been interrogated by x-ray diffraction, spectral ellipsometry, Hall measurements, and synchrotron-based hard x-ray photoemission. In this contribution, we will reveal how the optoelectronic material properties change upon annealing.

### **16 Study of the chemical and electronic properties of inorganic lead-free perovskites**

C. Hartmann, S. Gupta, X. Kozina, T. Kunze, G. Hodes, R. Félix, R.G. Wilks, D. Cahen, and M. Bär

$\text{CsSnX}_3$  (X=Br, Cl, I) inorganic perovskites are promising lead-free alternatives to the more common lead halides that currently push solar cell efficiency records. Their properties are, however, widely unknown. To identify the role of  $\text{SnF}_2$  (addition of which during synthesis improves performance), halide composition, and deposition route, corresponding chemical solution- and vacuum-deposited  $\text{CsSnBr}_3$  and  $\text{CsSnCl}_3$  thin films, respectively have been characterized by HAXPES.

## **17 Interface formation in SnS - based thin-film solar cells probed by hard x-ray photoelectron spectroscopy**

L. Köhler, R. E. Brandt, C. Yang, E. Handick, X. Liao, R. Félix, R. G. Wilks, R. G. Gordon, T. Buonassisi, and M. Bär

The interface formed upon atomic layer deposition of ZnO or ZnO:N onto intentionally oxidized SnS is studied using synchrotron-based hard x-ray photoelectron spectroscopy with different excitation energies. Significantly stronger changes in the chemical environment of Sn including the formation of a metallic phase and a more pronounced interface-induced band bending are observed upon deposition of the (undoped) ZnO compared to the ZnO:N contact layers.

## **18 Monitoring the formation of the Zn(O,S) / Cu(In,Ga)Se<sub>2</sub> interface**

T. Kunze, P. Jackson, D. Hariskos, A. Siebert, C. Hartmann, R. Felix, D. Gerlach, Y. Yamashita, S. Ueda, T. Chikyow, R. G. Wilks, W. Witte, M. Bär

Solar cells based on Cu(In,Ga)Se<sub>2</sub> thin films are considered to be an alternative to silicon-wafer based devices. In order to monitor the interface formation between Cu(In,Ga)Se<sub>2</sub> absorbers and Zn(O,S) - a non-toxic and more transparent substitute to the standard CdS buffer - buffer layer thickness series have been studied. To get a depth-dependent insight into the chemical interface structure HAXPES measurements have been performed at BESSY II (HIKE at KMC-1) and SPring-8 (BL15XU).

## **19 Impact of alkalis on the surface structure of Cu(In, Ga)Se<sub>2</sub> studied on in-system prepared model systems**

P. Yang, D. Greiner, J. Lauche, L. Köhler, C. Hartmann, X. Liao, T. Kunze, R. Félix, R. G. Wilks, Ch. Kaufmann, M. Bär

Post-deposition treatments (PDT) of Cu(In,Ga)Se<sub>2</sub> (CIGSe) absorbers with, e.g. sodium and potassium have recently enabled fabrication of photovoltaic devices with record performance. In order to systematically study the impact of alkali elements on the CIGSe structure, we have hard x-ray photoelectron and absorption spectroscopy at the HIKE endstation BESSYII KMC-1 to study model systems prepared in-system. Alkali PDT leads to significant modifications of the CIGSe surface properties.

## **20 In-system study of SnCl<sub>2</sub> precursor layers: First step towards the synthesis of Pb-free perovskites at EMIL**

Roberto Félix, Núria Llobera-Vila, Claudia Hartmann, Carola Klimm, Dan R. Wargulski, Manuel Hartig, Regan G. Wilks, and Marcus Bär

We present the first experimental results towards synthesizing Pb-free perovskite thin-films at the Energy Materials In-Situ Laboratory Berlin. A detailed study of vacuum-deposited SnCl<sub>2</sub> precursor layers of different thicknesses by x-ray photoelectron and Auger electron spectroscopy reveals significant changes in the chemical environment of Sn and Cl along the layer profile. These findings show the effect that substrate conditions – here (oxidized) Mo – can exert on the deposited material.

## 21 **MoO<sub>3</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> – an inherently unstable interface?**

Xiaxia Liao, Severin N. Habisreutinger, Sven Wiesner, Golnaz Sadoughi, Daniel Abou-Ras, Marc A. Gluba, Regan G. Wilks, Roberto Félix, Marin Rusu, Henry J. Snaith, and Marcus Bär

The MoO<sub>3</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> interface is systematically studied using synchrotron-based hard x-ray photoemission, scanning electron microscopy, energy-dispersive x-ray spectroscopy, and Raman spectroscopy. We find evidence for the presence of MoO<sub>3</sub>, MoO<sub>x</sub> (Mo<sup>5+</sup>), PbMoO<sub>4</sub>, PbI<sub>2</sub>, and CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> indicating that the MoO<sub>3</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> interface is unstable, possibly explaining the low power conversion efficiencies previously reported in corresponding solar cell devices.

## List of Participants

Abdi	Fatwa	fatwa.abdi@helmholtz-berlin.de
Al Amri	Amal	amal.amri@kaust.edu.sa
Alvarez	José	jose.alvarez@geeps.centralesupelec.fr
Anselmo	Ana Sofia	ana.anselmo@helmholtz-berlin.de
Arrozi	Ubed Sonai	ubed_sonai.fahrudin_arrozi@tu-dresden.de
Azarpira	Anahita	anahita.azarpira@helmholtz-berlin.de
Bachmann	Philipp	philipp.bachmann@fau.de
Bär	Marcus	marcus.baer@helmholtz-berlin.de
Bauer	Udo	udo.bauer@fau.de
Bienert	Ralf	ralf.bienert@bam.de
Braun	Artur	artur.braun@alumni.ethz.ch
Bulat	Natalia V.	natty.bu@yandex.com
Cao	Jie	jie.cao@helmholtz-berlin.de
Cerceau Isaak Neta	Augusta	augusta.cerceau@demet.ufmg.br
Cibura	Niklas	niklas.cibura@cec.mpg.de
Darowski	Nora	darowski@helmholtz-berlin.de
Di Carlo	Lidia	lidia.dicarlo@gmail.com
Dong	Kang	kang.dong@helmholtz-berlin.de
Drissi El-Bouzaidi	Mohcine	mohcinebouzaidi@gmail.com
Dubourdieu	Catherine	catherine.dubourdieu@helmholtz-berlin.de
Düll	Fabian	fabian.duell@fau.de
Efthimiopoulos	Ilias	iliefthi@gfz-potsdam.de
Emmler	Thomas	thomas.emmler@hzg.de
Erler	Xenia	xenia.erler@helmholtz-berlin.de
Felix	Roberto	roberto.felix_duarte@helmholtz-berlin.de
Feyerherm	Ralf	ralf.feyerherm@helmholtz-berlin.de
Gall	Stefan	gall@helmholtz-berlin.de
Gopal	Radha Krishna	rksingh.iiserk@gmail.com
Gorgoi	Mihaela	mihaela.gorgoi@helmholtz-berlin.de
Grepstad	Jostein Kvaal	jostein.grepstad@iet.ntnu.no
Guilherme Buzanich	Ana	ana.buzanich@bam.de
Habicht	Klaus	habicht@helmholtz-berlin.de
Hafed	Aimadedine	aimadedin@gmail.com
Handick	Evelyn	evelyn.handick@helmholtz-berlin.de
Härk	Eneli	eneli.haerk@helmholtz-berlin.de
Hartmann	Claudia	claudia.hartmann@helmholtz-berlin.de
Hoell	Armin	hoell@helmholtz-berlin.de
Hoffmann	Martin	martin.hoffmann@helmholtz-berlin.de
Hofmann	Jan Philipp	j.p.hofmann@tue.nl
Holub-Krappe	Elizabeta	holub-krappe@helmholtz-berlin.de
Jafta	Charl Jeremy	charl.jafta@helmholtz-berlin.de
Jung	Christian	christian.jung@helmholtz-berlin.de
Kato	Vincent	katovicent20@gmail.com
Kleider	Jean-Paul	jean-paul.kleider@geeps.centralesupelec.fr
Klingan	Katharina	katharina.klingan@fu-berlin.de
Kolbe	Michael	michael.kolbe@ptb.de
Köppen	Martin	m.koeppen@fz-juelich.de
Korzaledin	Mostafa	Korzaledin.mostafa@gmail.com
Kozina	Xeniya	xeniya.kozina@helmholtz-berlin.de
Krumrey	Michael	Michael.Krumrey@ptb.de

Kunze	Thomas	thomas.kunze@helmholtz-berlin.de
Laueremann	Iver	iver.laueremann@helmholtz-berlin.de
Lechner	Rainer T.	rainer.lechner@unileoben.ac.at
Lestari	Witri Wahyu	witri@mipa.uns.ac.id
Liao	Xiaxia	xiaxia.liao@helmholtz-berlin.de
Loos	Stefan	stefan.loos@fu-berlin.de
MacQueen	Rowan	rowan.macqueen@helmholtz-berlin.de
Mahale	Pratibha	pratibha.mahale94@gmail.com
Mahmood	Khalid	khalid_mahmood856@yahoo.com
Makarova	Anna A.	aa.makarova@yandex.com
Martin	Niklas	fvee@helmholtz-berlin.de
Martinez Hardigree	Josue F.	josue.martinezhardigree@physics.ox.ac.uk
Martynova	Yulia	y.martynova@fz-juelich.de
Matte	Herma Sun Siva R.	krishna@physik.hu-berlin.de
Mazzio	Katherine A.	katherine.mazzio@helmholtz-berlin.de
Melke	Julia	julia.melke@fmf.uni-freiburg.de
Mihailetchi	Valentin	valentin.mihailetchi@isc-konstanz.de
Mohammadi	Mohammad Reza	reza.mohammadi@fu-berlin.de
Montoro	Luciano Andrey	landrey.montoro@gmail.com
Mulazzi	Mattia	mmulazzi@physik.hu-berlin.de
Müller	Roland	Roland.Mueller@helmholtz-berlin.de
Niederhausen	Jens	jens.niederhausen@helmholtz-berlin.de
Ning	De	de.ning@helmholtz-berlin.de
Oh	Hyung-Suk	hyung-suk.oh@tu-berlin.de
Opitz	Andreas	Andreas.Opitz@hu-berlin.de
Papp	Christian	christian.papp@fau.de
Parvan	Vladimir	vladimir.parvan@helmholtz-berlin.de
Pasquini	Chiara	chiara.pasquini.cp@gmail.com
Pflüger	Mika	mika.pflueger@ptb.de
Prieto	Mauricio J.	prieto@fhi-berlin.mpg.de
Pryadchenko	Vasiliy V.	vvpryadchenko@sfedu.ru
Radnik	Jörg	Joerg.Radnik@bam.de
Radtke	Martin	martin.radtke@bam.de
Rai	Diby Prakash	dibyaprakashrai@gmail.com
Rander	Torbjörn	torbjorn.rander@win.tu-berlin.de
Raoux	Simone	simone.raoux@helmholtz-berlin.de
Reichardt	Gerd	gerd.reichardt@helmholtz-berlin.de
Rensmo	Håkan	hakan.rensmo@physics.uu.se
Roth	Christina	christina.roth@fu-berlin.de
Schavkan	Alexander	alexander.schavkan@desy.de
Schieda	Mauricio	mauricio.schieda@hzg.de
Schleusener	Alexander	alexander.schleusener@leibniz-ipht.de
Schneider	Claus M.	c.m.schneider@fz-juelich.de
Schorr	Susan	susan.schorr@helmholtz-berlin.de
Schultz-Wittmann	Oliver	oliver.schultz-wittmann@firstsolar.com
Schwarzkopf	Olaf	olaf.schwarzkopf@helmholtz-berlin.de
Seidel	Robert	Robert.Seidel@helmholtz-berlin.de
Shahraei	Ali	shahraei@ese.tu-darmstadt.de
Shaker	Maryam	maryam.shaker@helmholtz-berlin.de
Shashev	Yury	Yury.Shashev@bam.de
Siebert	Andreas	andreas.siebert@helmholtz-berlin.de
Sivakov	Vladimir	vladimir.sivakov@leibniz-ipht.de
Sokolov	Andrey	andrey.sokolov@helmholtz-berlin.de

Som	Tirtha	tirtha.som@helmholtz-berlin.de
Späth	Florian	florian.spaeth@fau.de
Staier	Florian	florian.staier@helmholtz-berlin.de
Stegemann	Bert	bert.stegemann@htw-berlin.de
Steinhauer	Johann	johann.steinhauer@fau.de
Svensson	Svante	Svante.Svensson@physics.uu.se
Tadout	Mohamed	tadout.mohamed@gmail.com
Udintseva	Margarita	Udintseva_m@mail.ru
Unterberg	Bernhard	b.unterberg@fz-juelich.de
Vargas-Barbosa	Nella Marie	nellamarievargas@gmail.com
Velasco Vélez	Juan Jesús	velasco@fhi-berlin.mpg.de
Vogel	Uwe	uwe.vogel@helmholtz-berlin.de
Wallacher	Dirk	dirk.wallacher@helmholtz-berlin.de
Wang	Yajie	yajie.wang@helmholtz-berlin.de
Wang	Qiankun	qiankun@physik.hu-berlin.de
Wansleben	Malte	malte.wansleben@ptb.de
Wegner	Berthold	berthold.wegner@helmholtz-berlin.de
Wiese	Martin	martin.wiese@ise.fraunhofer.de
Xi	Lifei	lifei.xi@helmholtz-berlin.de
Xiao	Ting	ting.xiao@helmholtz-berlin.de
Xiaoyan	Du	xiaoyan.du@fau.de
Yang	Penghui	penghui.yang@helmholtz-berlin.de
Zeier	Wolfgang	wolfgang.g.zeier@phys.chemie.uni-giessen.de
Zhou	Dong	dong.zhou@helmholtz-berlin.de

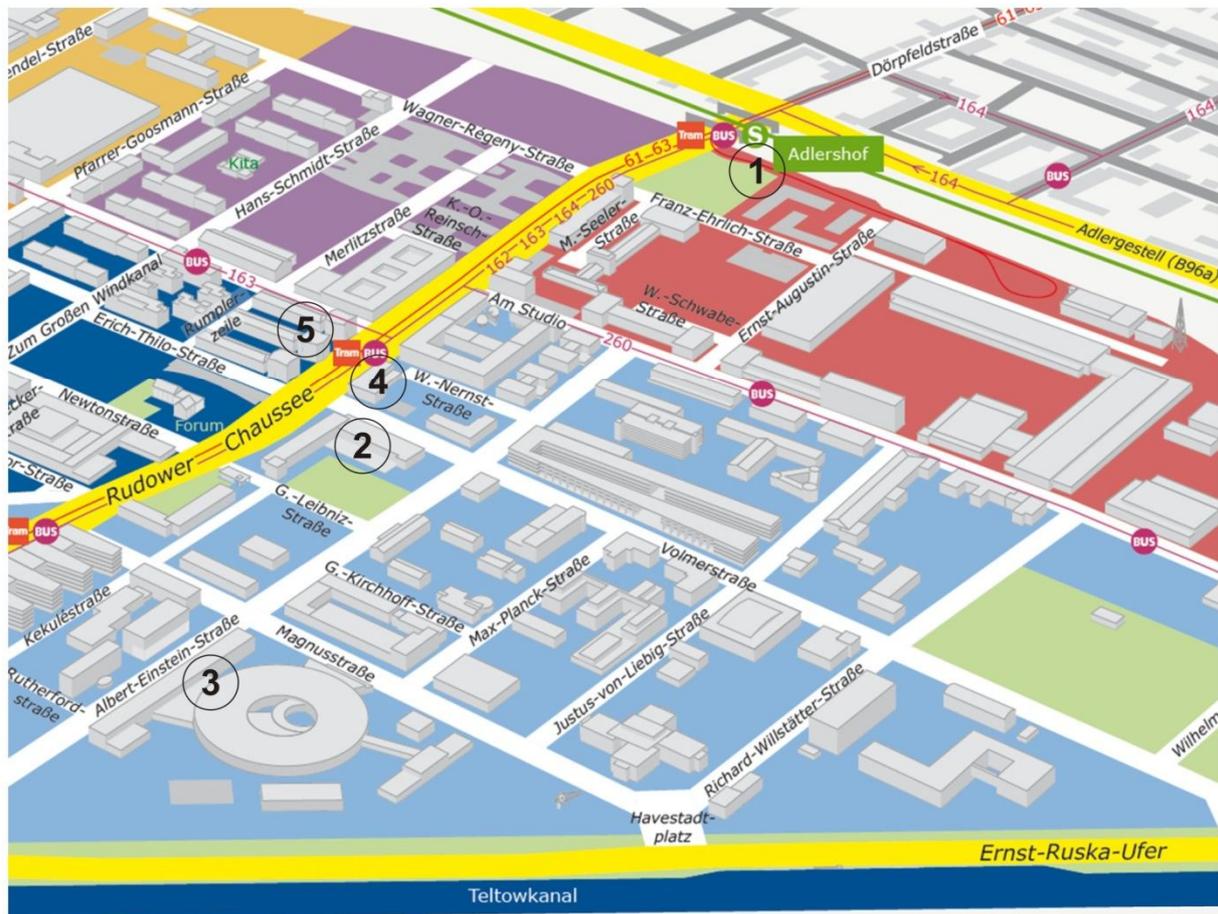
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## Site plan

### Helmholtz-Zentrum Berlin Wilhelm-Conrad-Röntgen Campus Adlershof



- ① Train Station Adlershof
- ② WISTA Centre: Registration 10th of October
- ③ HZB, BESSY II: Registration 11th of October

Poster Session

Hotels:

- ④ Dorint
- ⑤ Airport Hotel

**HZB, BESSY II**  
Albert-Einstein-Str. 15  
12489 Berlin

tel +49 (0)30 8062 - 12931  
fax +49 (0)30 8062 - 14746  
photons@helmholtz-berlin.de

## Confirmed Invited Speakers

Fraser Armstrong, University of Oxford, UK  
Neal Armstrong, University of Arizona, USA  
Marcus Bär, HZB, DE  
Christoph Brabec, Universität Erlangen, FAU, DE  
David Cahen, Weizmann Institute of Science, IL  
Petra de Jongh, Utrecht University, NL  
Antonio Facchetti, Polyera Corporation, USA  
Martin Hermle, Fraunhofer ISE, DE  
Daniil Itkis, Lomonosov Moscow State University, RU  
Jürgen Janek, Justus-Liebig-Universität Gießen, DE  
Axel Knop-Gericke, FHI, MPG, DE  
Norbert Koch, Humboldt Universität zu Berlin, DE  
Stefan Koller, VARTA Micro Innovation, AT  
Uli Lemmer, Karlsruher Institut für Technologie, DE  
Heiner Linke, Lund University, SE  
Emil List-Kratochvil, Humboldt Universität zu Berlin, DE  
Frank Renner, Hasselt University, BE  
Rutger Schlatmann, PVcomB, DE  
Wim Sinke, University of Amsterdam, NL  
Peter Strasser, Technische Universität Berlin, DE  
Andy Thomas, IFW Dresden, DE  
Eva Unge, Lund University, SE  
Roel van de Krol, HZB, DE  
Peter Wasserscheid, Universität Erlangen, FAU, DE  
Andreas Züttel, EPFL, CH

## Scientific Committee

Marcus Bär  
Klaus Lips  
Simone Raoux  
Bernd Rech  
Roel van de Krol  
Antje Vollmer

## Local Organizing Committee

Britta Höpfner  
Daniela Theile  
Florian Staier  
Antje Vollmer

## Meeting Venue

### 10th of October:

**Bunsen Saal, Adlershof con.vent. WISTA Centre**  
Rudower Chaussee 17  
12489 Berlin  
Germany

### 11th of October:

**Helmholtz-Zentrum Berlin für Materialien und Energie**  
Albert-Einstein-Str. 15  
12489 Berlin-Adlershof  
Germany  
[www.helmholtz-berlin.de](http://www.helmholtz-berlin.de)

## CONTACT

[antje.vollmer@helmholtz-berlin.de](mailto:antje.vollmer@helmholtz-berlin.de)

Further information and updates can be found at  
[http://www.helmholtz-berlin.de/user/workshops/energy/index\\_en.html](http://www.helmholtz-berlin.de/user/workshops/energy/index_en.html)

