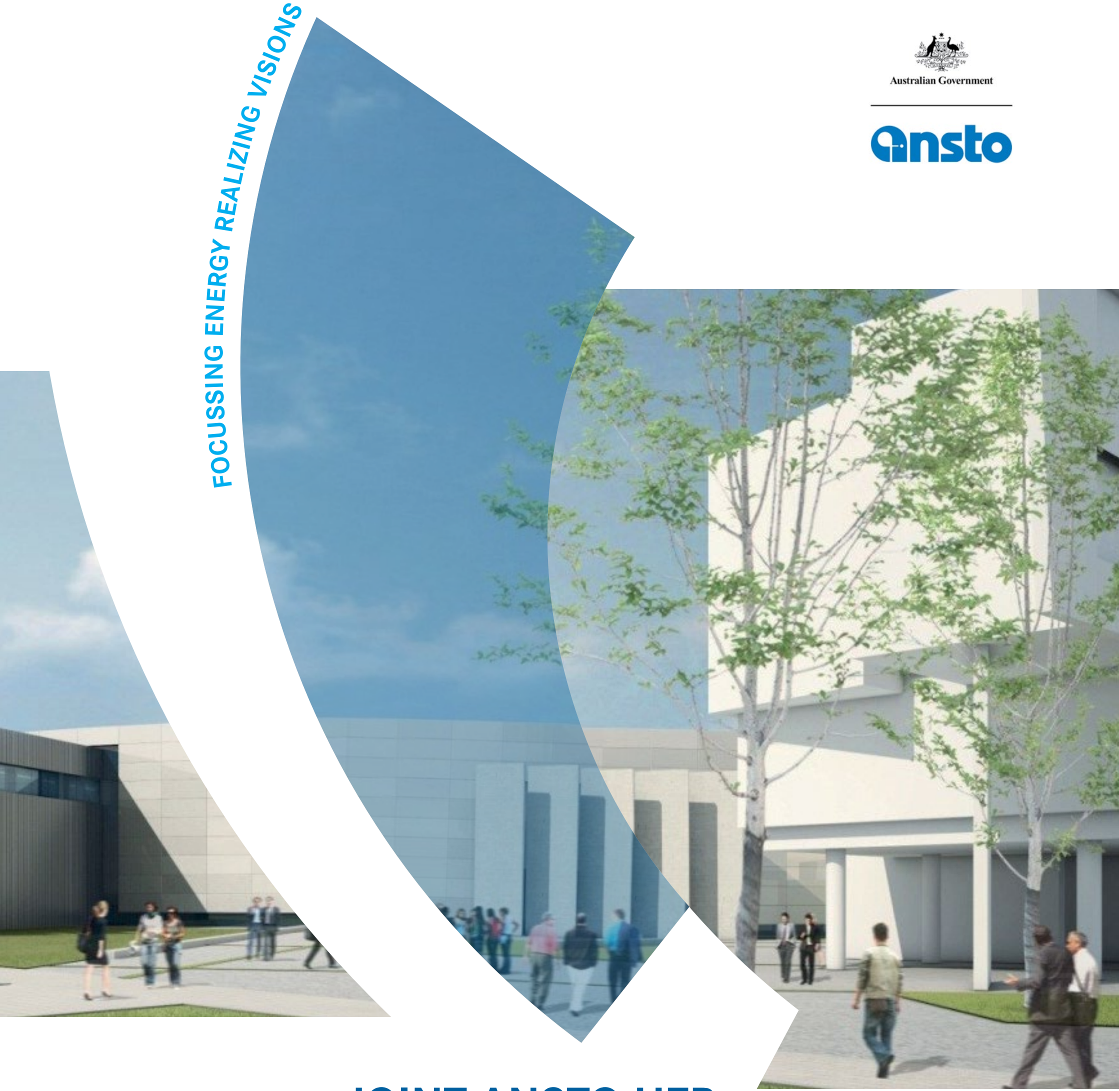
HZB Helmholtz Zentrum Berlin

Australian Government

ansto

FOCUSSING ENERGY REALIZING VISIONS



JOINT ANSTO-HZB WORKSHOP

March 7th, 2017
BESSY II Lecture Hall

Joint ANSTO-HZB Workshop

Perspectives for energy and materials science research with large scale facilities

7th March 2017
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
BESSY II Lecture Hall

In October 2016 the Australian Nuclear Science and Technology Organisation (ANSTO) and Helmholtz Zentrum Berlin für Materialien und Energie (HZB) signed an umbrella Memorandum of Understanding (MoU) to merge former independent efforts, provide principles for cooperation and establish scientific collaborations and staff exchange in the field of energy materials research with – but not only – advanced analytics and large scale facilities.

This workshop aims at exchanging information and perspectives of current research activities at ANSTO and HZB for further concretization of joint scientific projects of mutual benefit.

HZB Helmholtz Zentrum Berlin

Australian Government

ansto

Program

Tuesday, 7 March 2017		
WCRC Adlershof, **BESSY II, Lecture Hall**		
08:30-08.55	Meeting and registration at BESSY II Foyer	
09.00-09.15	**Welcome address:** **Prof. A. Kaysser-Pyzalla or Thomas Frederking, HZB Board of Directors** **Dr. Jamie Schulz, Leader of the Australian Centre for Neutron Scattering at ANSTO (*t.b.c.*)**	
09.15-10.50	**Session 1: Energy materials research with photons**	
	Chair:	Dr. Catalina Jiménez
	09.15-09.35	**Energy Materials Research at the Australian Synchrotron**
		Prof. Michael James (Head of Science at the Australian Synchrotron)
	09.40-10.00	**The energy materials in-situ lab EMIL at BESSY II**
		Prof. Klaus Lips
	10.05-10.25	**Photon-based characterization of energy materials in both the energy and time domain**
		Prof. Emad Aziz
	10.30-10.50	**Energy materials research with resonant microwave photons**
		Prof. Jan Behrends and Dr. Alexander Schnegg
10.50-11.10	Coffee break	
11.10-13.10	**Session 2: Energy materials research with neutrons**	
	Chair:	Dr. Roland Steitz
	11.10-11.30	**Energy-materials research using neutron scattering at ANSTO**
		Prof. Garry McIntyre, Research Leader at the Australian Centre for Neutron Scattering
	11.35-11.55	**Neutrons for spin liquids and functional materials in the FIT program**
		Prof. Bella Lake
	12.00-12.20	**Structure and dynamics of hybride perovskites: insights by neutron scattering**
		Prof. Susan Schorr
	12.25-12.45	**In-situ analysis with neutrons and photons of electrode materials for electrochemical energy storage**
		Dr. Sebastian Risse
	12.50-13.10	**Energy Materials and Neutron Reflectometry at ANSTO**
		Dr. Anton LeBrun (Instrument scientist at the OPAL neutron source)
13.10-14.00	Lunch	

14.00-15.50	**Session 3: Beamlines at BESSY II & user service**	
	Chair:	Dr. Alexander Schnegg
	14.00-14.35	**Research Opportunities at the New BR—GHT Beamlines at the Australian Synchrotron**
		Prof. Michael James
	14.40-15.00	**Experimental capabilities at BESSY II**
		Dr. Christian Jung
	15.05-15.25	**Research on topological insulators at the ARPES beamlines of BESSY II**
		Prof. Oliver Rader
	15.30-15.50	**User service, user involvement and quality management for user beamtime projects**
		Dr. Antje Vollmer
15.50-16:30	Coffee & Conclusion	

ABSTRACTS

Michael James – Australian Synchrotron

Energy Materials Research at The Australian Synchrotron

The Australian Synchrotron is one of Australia's premier research facilities and, at about $300 million, represents one of the biggest single investments in scientific excellence in the nation's history. Operated by the Australian Nuclear Science and Technology Organisation, the Australian Synchrotron produces intense beams of X-ray and infrared light at its ten experimental endstations, providing world-class research capabilities. Since commencing user operations in 2007 the Australian Synchrotron has become an integral part of the Australian and New Zealand research landscape, having supported over 35,000 user visits. To date the facility has generated more than 3000 peer reviewed journal articles, with a sizable proportion appearing in leading journals such as *Nature*, *Science*, *Advanced Materials*, *Physical Review Letters*, and *Proceedings of the National Academy of Science, USA*.

This presentation will highlight research performed on new energy materials at the Australian Synchrotron in collaboration with our staff, which has led to advances in the fields of organic photovoltaics and electronics, batteries, hydrogen storage systems, gas separation and carbon sequestration technologies, as well as other new classes of low-energy electronics.

Klaus Lips - Helmholtz-Zentrum Berlin

EMIL - a novel research platform for energy materials at the BESSY II synchrotron light source

A knowledge-based approach towards developing materials for energy conversion and storage application requires a fast and direct feedback between sophisticated analytics and state-of-the-art material processing facilities. At the Energy Materials In-situ Laboratory Berlin (EMIL) we achieve this by coupling synchrotron-based X-ray characterization techniques with relevant sample preparation techniques in one dedicated ultra-high vacuum (UHV) system which allows automated sample transfer within four minutes. EMIL is a joint project between Helmholtz-Zentrum Berlin and the Max Planck Society and will be fully operational in 2018. EMIL will provide light in an energy range from 70 – 10.000 eV which are distributed to five experimental endstations. EMIL consists of a 2000m2 large laboratory infrastructure with deposition, chemistry and spectroscopy labs as well as a cleanroom facility.

In this presentation, I will provide an overview of the analytic and material capabilities at EMIL and report on the status and timeline of the project. I will discuss the overall estimated performance and highlight how EMIL can trigger research opportunities for future user operation.

Emad F. Aziz - Helmholtz-Zentrum Berlin

Photon-Based Characterization of Energy Materials in Both the Energy and Time Domain

Photocatalytic processes occur in solution and/or at interfaces. To understand and thus improve photocatalytic functionalities, analytical probes sensitive in bulk-solution or at interfaces are vital. For this, we develop and apply X-ray-based analytical tools for **a complete characterization of the molecular - electronic and nuclear - structure of catalytical materials**. In my talk, I will present the photo-induced spin-flip in Fe(II) complexes represents an ultrafast phenomenon that has the potential to become an alternative to conventional processing and magnetic storage of information as an example for system studied by our team. We applied ultrafast XUV photoemission spectroscopy[1] to track the low-to-high spin dynamics in aqueous iron tris-bipyridine complex, $[Fe(bpy)_3]^{2+}$, by monitoring the transient electron density distribution among excited states with a femtosecond time resolution.[2]

References:
[1] Metje, J. et al. Monochromatization of femtosecond XUV light pulses with the use of reflection zone plates. Opt. Express 22, 10747 (2014).
[2] Moguilevski, A. et al. Ultrafast Spin Crossover in [FeII(bpy)3]2+: Revealing Two Competing Mechanisms by Extreme Ultraviolet Photoemission Spectroscopy. ChemPhysChem Early view (2017). doi:10.1002/cphc.201601396

Energy Materials Research with Resonant Microwave Photons

Jan Behrends, Alexander Schnegg, Klaus Lips

Berlin Joint EPR Lab

Unpaired electron spins provide unique probes for studying materials that are capable of producing or storing energy. These materials include e.g. organic and inorganic semiconductor energy convertors, catalytically active transition metal ion complexes and energy storage materials. Electron paramagnetic resonance (EPR) spectroscopy is the method of choice to gain information about function-determining paramagnetic states. The Berlin Joint EPR Laboratory (BeJEL) of Freie Universität Berlin and Helm-holtz-Zentrum Berlin für Materialien und Energie bundles cutting-edge experimental EPR facilities and expert knowledge available at the partner institutes for unique EPR studies in energy materials and devices. The experimental facilities include lab- and synchrotron-based EPR instrumentation for ex-situ and in-situ EPR experiments, cover-ing excitation energies from MHz to THz frequencies. After giving an overview about the different activities within BeJEL, the presentation will focus on recent examples of energy materials research based on advanced EPR techniques. Particular emphasis will be given to materials with applications in photovoltaics, spectral conversion, thermoe-lectrics and catalysis.

Energy-materials research using neutron scattering at ANSTO

Garry J McIntyre, Vanessa K Peterson, and Max Avdeev

Australian Centre for Neutron Scattering, ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia

As befits a national facility, the neutron-scattering science at the OPAL reactor at ANSTO is largely driven by the external user programme, through a peer-review proposal system for access to the neutron-beam instruments. Certain scientific themes, where neutrons offer distinct advantages, are also promoted within ANSTO, amongst which the research project *Functional Materials for Energy Devices and Systems*, led by Vanessa Peterson, and effectively a continuation of the highly successful *Energy Materials* project [1]. Of the six broad topics of focus: Hydrogen Production, Gas Storage and Separation, Fuel Cell Materials, Battery Materials, Thermoelectric Materials, and Solar Cell Materials, research into Battery Materials dominates, and has produced numerous pioneering results, including the first *in situ operando* studies of real batteries using neutron scattering. The magnetism theme [2] of the research project *Magnetism and Superconductivity*, coordinated by Max Avdeev, also includes research into magnetocaloric materials and the magnetic properties of battery materials, a knowledge of which aids fine-tuning of Density Functional Theory calculations to predict materials with improved performance.

This presentation will summarise current energy-materials research at ACNS within the context of the overall user programme.

References:

[1] http://www.ansto.gov.au/ResearchHub/OurInfrastructure/ACNS/CurrentResearch/ScientificProjects/EnergyMaterials/index.htm

[2] http://www.ansto.gov.au/ResearchHub/OurInfrastructure/ACNS/CurrentResearch/ScientificProjects/Magnetism/index.htm

Bella Lake - Helmholtz-Zentrum Berlin

Neutrons for spin liquids and functional materials in the FIT program

The Helmholtz Program “Future Information Technologies” (FIT) aims to perform basic research in topics relevant to new concepts for faster and more energy efficient computing and data storage in the medium to long-term future. Research areas include spin liquids whose topologically protected quantum states may provide stable qubits for quantum computers, unconventional superconductors, which hold promise for lossless electrical transport and multifunctional states which are relevant to data storage and switching. In this talk I will give some examples from different areas within the FIT program and then focus on the experimental search and identification of spin liquid states in quantum magnets.

Susan Schorr – Helmholtz-Zentrum Berlin

Structure and Dynamics of hybride perovskites: insights by neutron scattering

Organic (A) metal (B) halide (X) perovskites (ABX_3) are an enchanting class of semiconductor materials giving new possibilities of developing highly efficient, low-cost and stable single and multi-junction solar energy conversion devices. These compounds consist of an organic molecule i.e $CH_3NH_3^+$ (methylammonium abbreviated as MA), Pb on B-position and halides (I, Cl, Br) on X position. Compositional engineering is found to be a fruitful strategy for band gap tuning and obtaining hybride perovskites with enhanced optoelectronic properties.

To understand the origin of their PV performance, it is essential to first understand the crystal structures of the hybrid perovskites, characterized by structural phase transitions, considerable static or dynamic disorder, and unknown concentrations of various defects such as halogen anion or organic cation vacancies. The organic portion makes neutrons particularly useful in such investigations given their sensitivity to hydrogen and ability to distinguish clearly between carbon and nitrogen.

The presentation will show an overview of our studies on MAPI using complementary neutron and synchrotron X-ray powder diffraction as well as our first investigations of the molecule dynamics by quasielastic neutron scattering (QENS)

We are aim to extend our studies to solid solutions obtained by cation and anion mutation to gain understanding of the interrelationship of static and dynamic structure of the material.

In-Situ Analysis with Neutron and Photons of Electrode Materials for electrochemical Energy Storage

S. Risse[1], B. Seidlhofer[1], C. Jafta[1], M.Trapp[1], N. Kardjilov[2], A. Hilger[2], I. Manke[2] and M. Ballauff[1]

1 Institute of Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany
2 Institute of Applied Materials, Helmholtz-Zentrum Berlin, Germany

Lithium ion batteries are the most common secondary batteries that are used in mobile devices, automotive applications or as intermediate energy storage system in households and industry. However, the immense research in this field has pushed this storage system close to its theoretical energy density limits. Further progress in higher energy densities relies on the utilization of novel electrode concepts at the anode and cathode side. These new next-generation electrodes like silicon anodes and sulfur cathodes with nine and five times higher energy densities[1,2], respectively, are promising candidates for the post lithium ion era.

However, these new concepts are challenging due to their complex chemistry and unsolved capacity fading issues. Therefore it is important to employ sophisticated analysis methods to study these systems *in-situ*. This will yield new insights into the underlying degradation mechanisms. Sulfur cathodes were analyzed with a novel operando cell to study macroscopic structure formations with *operando* X-ray radiography.[3] The lithiation and delithiation process in silicon anodes was investigated with *in-situ* neutron reflectometry.[4] The results of these two experiments will be discussed in this presentation.

References:
[1] *Chem. Rev. 114*, 11751–11787 (2014)
[2] *J. Power Sources 202*, 308–313 (2012)
[3] *PCCP 18*, 10630 (2016)
[4] *ACS Nano 10*, 7458–7466 (2016)

Energy Materials and Neutron Reflectometry at ANSTO

Anton P. Le Brun, Andrew R.J. Nelson, Frank Klose, and Stephen A. Holt

Australian Centre for Neutron Scattering, ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia

Neutron reflectometry is a powerful technique for studying the thickness and composition of films and multilayer systems. ANSTO currently has one operating reflectometer (PLATYPUS) and another that is currently early in the installation stage (SPATZ, formerly BioRef from HZB). There is also a suite of supporting infrastructure for characterisation and fabrication including: X-ray reflectometry, imaging ellipsometry, spin-coating, Langmuir-Blodgett and Langmuir-Schaefer dipping, quartz-crystal microbalance with dissipation, etc. The combination of neutron instrumentation and ancillary equipment represents a world-class facility for studying thin-film materials, particularly those with energy applications. The scientific community have used the reflectometry facilities at ANSTO in collaboration with the reflectometry instrument scientists to characterise a range of energy materials including organic light-emitting diodes (OLEDs) [1, 2], hydrogen absorption [3], magnetic materials [4], and biopolymers [5]. The presentation will provide an overview of research achievements to date in characterising energy materials using reflectometry at ANSTO.

References:

[1] McEwan, JA; Clulow, AJ; Shaw, PE; Nelson, A; Darwish, TA; Burn, PL and Gentle, IR, Diffusion at interfaces in OLEDs containing a doped phosphorescent emissive layer, Advanced Materials Interfaces 3(17), 1600184 (2016)

[2] Smith, ARG; Lee, KH; Nelson, A; James, M; Burn, PL and Gentle, IR, Diffusion - the Hidden Menace in Organic Optoelectronic Devices, Adv. Mater. 24(6), 822-826 (2012)

[3] Callori, S; Rehm, C; Causer, G; Kostylev, M and Klose, F, Hydrogen Absorption in Metal Thin Films and Heterostructures Investigated in Situ with Neutron and X-ray Scattering, Metals 6(6), Art. No. 125 (2016)

[4] Callori, SJ; Bertinshaw, J; Cortie, DL; Cai, JW; Le Brun, AP; Zhu, T and Klose, F, 90° magnetic coupling in a NiFe/FeMn/biased NiFe multilayer spin valve component investigated by polarized neutron reflectometry, J. Appl. Phys. 116(3), Art. No. 033909 (2014)

[5] Su, J; Raghuwanshi, VS; Raverty, W; Garvey, CJ; Holden, PJ; Gillon, M; Holt, SA; Tabor, R; Batchelor, W and Garnier, G, Smooth deuterated cellulose films for the visualisation of adsorbed bio-macromolecules, Sci Rep 6, 36119 (2016)

Michael James –Australian Synchrotron

Research Opportunities at the New BR-GHT Beamlines at the Australian Synchrotron

The Australian Synchrotron is one of Australia's premier research facilities and, at about AUD$300 million, represents one of the biggest single investments in scientific excellence in the nation's history. Despite this substantial investment, an enviable record in machine reliability as well as excellent scientific productivity, the Australian Synchrotron remains one of the most undercapitalised facilities in the world. Achieving first light in 2006 and first users in 2007, the Australian Synchrotron currently only operates its original suite of 10 beamlines.

Following extensive consultation with the User Community, the Science Case for the Phase II beamlines at the Australian Synchrotron was finalised in 2010. The conceptual designs for several of the priority beamlines were further refined in 2012, before a hiatus in the planning for new beamlines while the ongoing operational funding of the facility was settled.

2016 saw a substantial re-engagement with respect to new beamline development; made possible by the Australian Commonwealth Government's AUD$520 million, 10 year operating funding package for the Australian Synchrotron. The BR-GHT campaign was subsequently launched, with the aim of securing AUD$114 million to fund the construction of 8 new beamlines. It is expected that the BR-GHT program will commence later this year.

This presentation will detail the beamlines that form the BR-GHT suite of instruments at the Australian Synchrotron; discuss their conceptual designs and areas of scientific impact.

Christian Jung - Helmholtz-Zentrum Berlin

Experimental Capabilities at BESSY II

The BESSY II synchrotron radiation source is a 3rd-generation 1.7 GeV storage ring with high average brilliance serving an international user community with about 2,800 user visits per year. BESSY II beamlines focus to the VUV and soft-X-ray photon range. The beamlines are operated by HZB as well as in cooperation with strategic partners. The source and the instrument suite are very versatile and deliver photons at a high average brilliance. BESSY II provides high energy (~meV), spatial (10 nm) as well as temporal (sub-picosecond) resolution and full polarization control at repetition rates of up to 500 MHz. At dedicated beamlines access to very low (<0.01 eV) and high (>10 keV) photon energies permits special experiments, some beamlines are optimized for THz or single-bunch operation. Based on a longstanding experience in the design and development of undulators and optical beamline components, BESSY II was able to develop tailor made beamline solutions for specific experimental requirements. For dynamic spectroscopy the transmission could be improved by up to a factor of 5 using a novel zone plate monochromator design. For EMIL, the Energy Materials In-situ Laboratory, a novel beamline design was developed to cover the energy range from soft to hard X-rays.

Oliver Rader - Helmholtz-Zentrum Berlin

Research on topological insulators at the ARPES beamlines of BESSY II

Topological matter is of high current interest as the bestowal of the Nobel prizes 2016 shows. Generally, a topological insulator features a metallic surface protected by time-reversal symmetry and an isulating bulk. In this talk we introduce the properties of three-dimensional topological insulators through their signatures in spin- and angle-resolved photoelectron spectroscopy obtained at the BESSY II endstations ARPES1^2, ARPES1^3, and PHOENEXS. We discuss the magnetic functionalization of topological insulators and the conditions for the creation of magnetic band gaps by impurities as they are a necessary condition for the quantum anomalous Hall effect. Topological insulators are a pure band structure effect, however, electron correlation would add interesting aspects. SmB6 has meanwhile been established as the first correlated topological insulator and the first topological Kondo insulator. We show, however, with the help of data taken at ultrahigh resolution at T=1 K with the ARPES 1^3 instrument that the existing ARPES evidence does not support topological surface states and that the surface metallicity of SmB_6 has a simple, topologically trivial origin. So-called topological crystalline insulators are more vulnerable systems where surface states are protected by mirror symmetries only instead of time-reversal symmetry. We show that the system $Pb_{1-x}Sn_xSe$ can be driven by doping into a topological quantum phase transition from mirror- to time-reversal symmetry protection.

Antje Vollmer – Helmholtz-Zentrum Berlin

User Service, User Involvement and Quality Management for User Beamtime Projects at HZB

Currently BESSY II offers 38 beamlines in user operation with another 7 to become operational in the near future[1]. In addition to the synchrotron based infrastructures HZB provides so called CoreLabs[2], operated as multi-user platforms for external academic and industrial partners and a Lab Cluster for sample preparation and charaterisation.

Altogether HZB welcomes roughly 1800 users per year in more than 3000 user visits.

In this presentation we will discuss the administrative and scientific user service as well as a newly implemented Quality Management[3] for user beamtimes based on different feedback schemes and key indicators to improve the quality of user support and user infrastructures.

A major emphasis is given to the involvement of our users. In addition to regular user meetings, an elected user committee and informal user coffees with lectures on new developments and possibilities, HZB has established a series of foresight workshops[4]. They are designed to offer a continuous discussion platform for future projects and research activities in concert with current and future users from universities, research institutes, and industry to identify future scientific fields as well as expectations, needs, and requirements for cutting edge science with synchrotron radiation.

References:
[1] https://www.helmholtz-berlin.de/user/experimental-infrastructures/instruments-photons/index_en.html
[2] https://www.helmholtz-berlin.de/quellen/corelabs/index_en.html
[3] https://www.helmholtz-berlin.de/pubbin/vademecumdatei?did=331
[4] https://www.helmholtz-berlin.de/user/workshops/index_en.html

NOTES

We are researching new energy materials that will convert and store energy more efficiently and with a smaller ecological footprint than ever before, for example solar cells, thermoelectrics and solar fuels. The photon source BESSY II is an ideal place for studying thin film systems and our CoreLabs an excellent place for producing and analysing them. We make these infrastructures available to researchers from everywhere in the world. Industrial companies are also very welcome. Our internationality, creativity and pursuit of new solutions are what set us apart.

When are you coming to visit?
helmholtz-berlin.de

FOLLOW US

JOINT ANSTO-HZB WORKSHOP

CONTACT
steitz@helmholtz-berlin.de
catalina.jimenez@helmholtz-berlin.de