EIGHTH JOINT BER II AND BESSY II USERS MEETING

Dec. 7-9, 2016

Key Note Lecture:
Eduardo Higino da Silva Neto
(University of California Davis)
Public Lecture:
Lídice Vaillant Roca (University of La Habana)

- Synchrotron Instrumentation Day
- Young Scientists Sessions
- Science Day
- Vendor Exhibition
- Poster Session
- Neutron Instrumentation Day

Invited talks:
Stefan Kaskel *(TU Dresden)*
Hiroki Wadati *(University of Tokyo)*
Markus Morgenstern *(RWTH Aachen)*
Joachim Reichert *(TU München)*
Erik Vesselli *(University of Trieste)*
Oliver Daumke *(MDC Berlin)*
Hans-Joachim Elmers *(Johannes Gutenberg Universität)*
Dennis Wiedemann *(TU Berlin)*
Annette Pietzsch *(HZB)*
Christina Roth *(FU Berlin)*

Satellite Workshops:

- **Challenges in diffraction data processing – How to get the most out of your data (Dec. 9)**
- **HFM/EXED Session (Dec. 9)**

December 7 to 9, 2016
Wilhelm-Conrad-Röntgen Campus, Berlin-Adlershof
and WISTA and
Lise-Meitner-Campus, Berlin-Wannsee

http://hz-b.de/um2016

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Dear friends and users,

Welcome to the 8th Joint BER II and BESSY II User Meeting of HZB, which brings together users from our neutron and synchrotron sources at our sites in Berlin Wannsee and Adlershof.

In 2016 the synchrotron source BESSY II succeeded to further enhance its performance for both well settled and also novel experiments. In its very unique way BESSY II combines the constant, stable and reproducible flux of the multi bunch train with tailored filling patterns and specific bunch characteristics for various types of timing experiments. This technique of a simultaneous accommodation of experiments with very specific demands has been extended in 2016. The pseudo single bunch capability of the PPRE bunch has been extended to the low alpha mode. In addition a novel low current 2ps short bunch is provided as a milestone towards BESSY VSR. On the Sundays of the single bunch week a four bunch mode with higher current increases the repetition rate from 1.25 MHz to 5MHz.

On 31st of October 2016, the official opening of EMIL@BESSY II was celebrated, in the presence of the honorable Federal Minister for Science and Technology, Prof. Johanna Wanka, the president of the Helmholtz Association Prof. Otmar Wiestler and high representatives from the Max-Planck Society. With the new soft X-ray undulator being in place, the last part of the beamline was installed by Prof Wanka during the inauguration ceremony, and thus the soft branch of EMIL@BESSY II is ready for commissioning. EMIL@BESSY II is part of HZBs suite of CoreLabs. These newly implemented laboratories will complement the synchrotron infrastructures and provide state-of-the-art laboratories as well as unique equipment and will serve the wider scientific community by offering services and access to external academic and industrial users. The X-ray CoreLab covers different modern X-ray diffraction methods focusing on in-situ studies of phase transitions and texture analysis. The microscopy CoreLab, participating in the ZEISS labs@location program, enables cutting-edge research on novel materials with the most modern ZEISS electron microscopes available. The HySPRINT CoreLab will focus on hybrid materials and components based on silicon and perovskite crystals used for energy conversion in photovoltaics as well as for solar hydrogen production.

Several other important projects to improve the performance of our beamlines and end stations were finalized including the LowDosePES station with its MHz chopper and laser running, the coincidence ARTOF station coESCA, and the relocation of the XM X-ray Microscope. Furthermore the U125-RGBL undulator beamline as well as the PEAXIS station combining RIXS and PES on solid and liquid samples will be opened to friendly users soon. The planning of the two projects ENERGIZE, a beamline dedicated to research on hybrid materials and energy efficient technologies, as well as METRIXS, a high resolution state-of-the-art spectrometer for resonant inelastic X-ray scattering, is in its final phase.

The series of Foresight Workshops which started in 2014 was continued this year with an especially well attended workshop on Energy Materials Research. The aim was to encourage a dialogue between the current and future users from universities, research institutes, and industry. The workshop assembling 250 participants brought new ideas and impulses on the future needs of the international community working on energy materials. The first six Foresight Workshops with altogether more than 880 participants covered the topics “Tender X-Rays”, Pico-to-femto - time resolved studies”, “Imaging” at BESSY II, “THz-to-Soft X-Rays”, “Tender X-Rays in MX” and “Energy Materials Research”.

A Quality Management system has been implemented to further improve the user support and to optimize the full process of user beamtime projects at BESSY II. All procedures necessary to enable a successful user visit have been visualized and structured promoting transparent processes that are open for further improvement. The Quality Management of the user service embraces BESSY II, the experimental infrastructures and all processes and people involved. Major tasks in our user service comprise high scientific output, outstanding infrastructure, high user satisfaction and further user demands. To meet these challenges, to assure a transparent access and to guarantee the best operation of the facilities, monitoring and optimizing all procedures is prerequisite which significantly relies on feedback from and communication with our users.

The neutron source BER II was operating with 10 neutron scattering instruments in 2016, including the unique HFM/EXED instrument, providing the strongest continuous magnetic field for neutron scattering worldwide. Implementation of a new inelastic option at HFM/EXED is in progress and will be available for users in 2017. Additionally the upgraded time-of-flight spectrometer NEAT is now in final commissioning and is starting regular user operation in 2017 as well.

This year’s Joint User Meeting is highlighted by the keynote lecture by Eduardo Higino da Silva Neto from the University of California, Davis on the “Electronic order in High-TC cuprate superconductors” and the public lecture by Lídice Vaillant Roca from the University of La Habana on “Solar Energy in an Emerging Country, Perspectives and the Need for International Cooperation”. The Verein Freundeskreis Helmholtz-Zentrum Berlin e.V. will bestow the Innovation Award and the Ernst-Eckart-Koch Prize. The Science Day on Thursday is concluded by a poster session accompanied by the traditional “Berlin Buffet”, kindly sponsored by the companies represented in the industrial exhibition. The Synchrotron Day and the Neutron Day each have a special highlight with a young scientist session. The User Meeting is accompanied by two satellite workshops on “HFM/EXED” in Wannsee and on “Challenges in diffraction data processing” in Adlershof.

We hope all these meetings will stimulate your interest in photons and neutrons research and initiate fruitful discussions and 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

Contents

Wednesday, December 7th, 2016 :
Young Scientist and Synchrotron Day

Wilhelm-Conrad-Roentgen Campus
Albert-Einstein-Str. 15
Rudower Chaussee 17
12489 Berlin

13:30 – 18:00	**Registration and Vendor Exhibition**	WISTA Centre
14:00 – 15:50	**Synchrotron Session** *(Chair: Christian Jung)*	Bunsen Auditorium
14:00	*Thomas Frederking (HZB)* **Welcome**	
14:10	*Andreas Jankowiak (HZB)* **Accelerator Operation and Projects @ HZB**	
14:30	*Alexander Föhlisch (HZB)* **BESSY II: Photon Science and Instrumentation**	
14:50	*Simone Raoux (HZB)* **Status of Energy Materials In-situ Lab (EMIL) at BESSY II**	
15:10	*Emad Flear Aziz (HZB)* **High-Resolution Spectrometer PEAXIS at BESSY II: Wide-Q-Range RIXS and ARPES Measurements on Solids, Solutions and at Interfaces**	
15:30	*Klaus Kiefer (HZB)* **Sample Environment at BESSY II**	
15:50 – 16:05	**General Discussion**	Bunsen Auditorium
16:05 – 16:30	**Coffee Break**	WISTA Centre
16:30 – 18:00	**Young Scientist Session** *(Chair: Benedetta Casu)*	Bunsen Auditorium
16:30	*Eva Absmeier (FU Berlin)* **Molecular control mechanisms in the Brr2 RNA helicase for efficient and regulated splicing**	
16:45	*Stefan Permien (CAU Kiel)* **What happens structurally and electronically during the Li Conversion Reaction of $CoFe_2O_4$ Nanoparticles: An Operando XAS and XRD Investigation**	
17:00	*Julia Maibach (Uppsala University)* **Buried Interfaces in Lithium Ion Batteries Probed with HAXPES**	
17:15	*Siobhan McKeown Walker (Universite de Genève)* **ARPES studies of the STO (001) 2DEG**	
17:30	*Marein Rahn (University of Oxford)* **All-in/all-out magnetic order in rare earth iridates**	
17:45	*Elmar Kataev (M.V. Lomonosov Moscow State University)* **Oxygen reduction reaction on graphene in Li-air batteries**	
18:00-19:00	**Classic curried sausage with "Schrippen" and beer**	WISTA Centre

Thursday, December 8th, 2016 : Science Day

Wilhelm-Conrad-Roentgen Campus
Albert-Einstein-Str. 15
Rudower Chaussee 17
12489 Berlin

9:00 – 16:00	**Vendor Exhibition**	WISTA Centre
8:30 – 9:30	**Registration and Poster Set-up**	WISTA Centre
9:30 – 9:40	**Opening** *Anke Kaysser-Pyzalla (HZB)*	Bunsen Auditorium
9:40 – 10:10	**Key Note Lecture** *(Chair: Carolin Schmitz-Antoniak)* *Eduardo Higino da Silva Neto (University of California, Davis)* **Electronic Order in High-T_C Cuprate Superconductors**	
10:10 – 10:40	**Coffee Break and Vendor Exhibition**	WISTA Centre
10:40 – 12:20	**Oral Presentations I** *(Chair: Emil J.W. List-Kratochvil)*	Bunsen Auditorium
10:40	*Stefan Kaskel (TU Dresden)* **In situ-observation of novel switching phenomena in highly porous Metal-Organic Frameworks**	
11:00	*Hiroki Wadati (University of Tokyo)* **Photoinduced demagnetization and insulator-to-metal transition in ferromagnetic insulating $BaFeO_3$ thin films**	
11:20	*Markus Morgenstern (RWTH Aachen)* **ARPES measurements of the ferroelectric bulk Rashba system GeTe**	
11:40	*Joachim Reichert, (TU München)* **Bisphenol A on Cu(111) and Ag(111): From Chemical Reactivity to Rotor Arrays**	
12:00	*Erik Vesselli (University of Trieste)* **Reverse Water-Gas Shift or Sabatier Methanation on Ni(110)? Stable Surface Species at Near-Ambient Pressure**	
12:20 – 13:30	**Lunch Break**	(Canteens on site)
13:30 – 15:10	**Oral Presentations II** *(Chair: Susan Schorr)*	Bunsen Auditorium
13:30	*Oliver Daumke (MDC Berlin)* **Structural studies of molecular machines**	
13:50	*Hans-Joachim Elmers (Johannes Gutenberg Universität)* **Multi-MHz time-of-flight electronic bandstructure imaging of graphene on Ir(111)**	
14:10	*Dennis Wiedemann (TU Berlin)* **Diffusion Pathways in Ion Conductors: Making the Most of Neutron-Diffraction Data**	

14:30	*Annette Pietzsch (HZB)* **Ground state potential energy surfaces around selected atoms from resonant inelastic x-ray scattering**	
14:50	*Christina Roth (FU Berlin)* **Characterization of electrocatalysts using a combination of XAS and DRIFTS**	
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15:50 – 17:00	**Bestowal of Prizes: Friends of Helmholtz-Zentrum Berlin e.V.** *(Chair: Mathias Richter)*	Bunsen Auditorium
17:00 – 18:00	**Public Lecture** *(Chair: Francesco Allegretti)* *Lídice Vaillant Roca (University of La Habana)* **Solar Energy in an Emerging Country, Perspectives and the Need for International Cooperation**	Bunsen Auditorium
18:00 – 20:00	**Poster Session**	(BESSY II Experimental Hall)
20:00	**Berliner Buffet and Poster Prize** (sponsored by the companies participating in the vendor exhibition)	(BESSY II Foyer)

Friday, December 9th, 2016:
Young Scientist and Neutron Day

Lise-Meitner Campus
Hahn-Meitner-Platz 1
14109 Berlin

8:30-9:00	**Registration**	(LMC-Foyer and Café Jahn)
9:00 – 9:50	**Neutron Session** *(Chair: Klaus Habicht)*	(Lecture Hall)
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9:10	*Sebastian Risse (HZB)* **In-Situ Neutron Analysis of Electrode Materials for electrochemical Energy Storage**	
9:30	*Katharina Fritsch (HZB)* **Structure and transport properties in thermoelectric skutterudites**	
9:50 – 11:05	**Young Scientist Session** *(Chair: Susan Schorr)*	(Lecture Hall)
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10:05	*Sandra Cabeza (BAM)* **Load partition and damage characterization of cast $AlSi_{12}CuMgNi$ alloy with one- and two ceramic reinforcements**	
10:20	*Simon Krause (TU Dresden)* **Neutrons shed light on methane adsorption mechanism in a series of highly porous metal-organic frameworks**	
10:35	*Alsu Gazizulina (Universität Zürich)* **Study of the structure and magnetic interactions in dimer system $Ba_{(3-x)}Sr_xCr_2O_8$**	
10:50	*Simone Mascotto (Universität Hamburg)* **Distribution of S in C-S nanocomposites analyzed by small-angle scattering methods**	
11:05 – 11:25	**Coffee Break**	(Café Jahn)
11:25 – 12:45	**HFM/EXED Session** *(Chair: Bella Lake)*	(Lecture Hall)
11:25	*Oleksandr Prokhnenko (HZB)* **Current status of HFM-EXED facility and its upgrade**	
11:45	*Matej Pregelj (Institut "Jozef Stefan")* **Pursuit of spin nematicity in s=1/2 frustrated zigzag chain beta-$TeVO_4$**	
12:05	*Karel Prokes (HZB)* **Electronic properties of $U(Ru_{0.92}Rh_{0.08})_2Si_2$ in high magnetic fields**	
12:25	*Ted Forgan (University of Birmingham)* **Field-dependent superconducting anisotropy and Pauli-paramagnetism in $YBa_2Cu_3O_7$ studied by time-of-flight small-angle neutron scattering from vortices in high fields**	
12:45 – 14:15	**Poster Session and Lunch**	(Café Jahn)
14:15	**HFM/EXED Tour**	(Café Jahn)

Abstracts of the Young Scientist Session at the Synchrotron Day

Wednesday, 7th of December

E. Absmeier 07.12.16, 16:30

Molecular control mechanisms in the Brr2 RNA helicase for efficient and regulated splicing

E. Absmeier[1], J. Wollenhaupt[1], S. Mozaffari-Jovin[2], C. Becke[1], C.-T. Lee[3], M. Preussner[1], U. Stelzl[4], F. Heyd[1], H. Urlaub[3], R. Lührmann[2], K. F. Santos[1], M. C. Wahl[1]

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The Ski2-like RNA helicase, Brr2, mediates disruption of the U4/U6 di-snRNP during spliceosome activation, and its activity has to be tightly regulated. While previous analyses have revealed how the helicase region of Brr2 is built from an active N-terminal and an inactive, regulatory C-terminal helicase cassette,[1] little attention has been paid to the structure and function of Brr2's ca. 500-residue N-terminal region (NTR). We present a high-resolution crystal structure of a non-canonical PWI domain[2] contained in the Brr2 NTR and a medium-resolution structure of full-length Brr2 in complex with the Jab1/MPN (Jab1) domain of the spliceosomal master regulator Prp8.[3] These structures show that the Brr2 NTR encompasses two folded domains and adjacent linear elements that clamp and interconnect the helicase cassettes. Stepwise truncations of the NTR lead to a stepwise increase in Brr2's RNA-binding, RNA-stimulated ATPase and RNA unwinding activities, and an increased preference for ATPγS over ADP binding. Trends in nucleotide binding, RNA binding, ATPase and helicase activities of the Brr2 NTR truncations are fully rationalized by the full-length Brr2 crystal structure, demonstrating that the NTR auto-inhibits Brr2 via substrate competition, conformational clamping and by gearing Brr2 towards a preference for ADP binding. The latter mechanism is supported by crystal structures of a Brr2 variant that lacks almost the complete NTR in the apo-state and bound to various nucleotides. In addition, NTR truncations are associated with reduced cell viability, less efficient pre-mRNA splicing, weaker association of Brr2 with U4/U6•U5 tri-snRNP and increased non-canonical disruption of the tri-snRNP in vivo. However, Brr2 is not only regulated by intra-molecular factors, but is also modulated by protein co-factors, such as the Prp8 Jab1 domain. The Jab1 domain can act as an inhibitor or activator of Brr2, depending on the insertion of its intrinsically unstructured tail into the Brr2 RNA binding tunnel.[4] Crystal structure analysis in combination with systematic in vitro RNA binding and unwinding studies revealed an intricate cross-talk between the two inhibitory mechanisms established via the cis-acting NTR and the trans-acting Jab1 domain. Together, our results reveal a complex system of regulatory mechanisms that fine-tune Brr2 activities during splicing.[5]

References:
[1] Proc. Natl. Acad. Sci. 109, 17418 (2012).
[2] Acta Crystallogr. D Biol. Crystallogr. 71, 762 (2015).
[3] Genes Dev. 29, 2576 (2015).
[4] Science 341, 90 (2013).
[5] Cell Cycle (in press).

S. Permien 07.12.16, 16:45

What Happens Structurally and Electronically during the Li Conversion Reaction of $CoFe_2O_4$ Nanoparticles: An Operando XAS and XRD Investigation

S. Permien[1], S. Indris[2], U. Schürmann[3], L. Kienle[3], S. Zander[4], S. Doyle[5], W. Bensch[1]

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Today's portable consumer electronics and electronic vehicles are under development and demand for new battery materials with higher energy density. The need to identify lithium battery anodes consisting of new materials exhibiting high energy density has intensified the research on reversible so-called conversion reactions between lithium and oxidic spinel materials such as, *e.g.*, $CoFe_2O_4$. *Operando* nondestructive synchrotron X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) were applied to directly determine the complex reaction mechanisms occurring during discharge and charge processes. Distinct reaction mechanism steps related to different electrochemical features of nanosized $CoFe_2O_4$ as the anode material are elucidated. The different discharge steps include uptake of a small fraction of Li into an amorphous layer covering the particles, the transformation of the spinel structure into a NaCl-like structure, and the formation of nanosized metallic Co and Fe embedded in a Li_2O matrix. The metals are oxidized to form Co^{2+} and Fe^{3+} during charging. The reaction $Fe^{3+} \leftrightarrow Fe^0$ is observed for many discharge/charge processes, whereas the oxidation of Co to Co^{2+} significantly declines during cycling, partially contributing to the capacity loss that occurs during cycling. The results demonstrate the importance of operando investigations on Li anodes for next-generation Li batteries, providing fundamental insights that are required to further improve their performance.[1]

References:

[1] Chemistry of Materials 28, 434 (2016).

J. Maibach 07.12.16, 17:00

Buried Interfaces in Lithium Ion Batteries Probed with HAXPES

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Lithium-ion batteries are nowadays commercialized and widely used but some of the underlying processes within the battery such as the formation of the solid electrolyte interphase (SEI) are not yet fully understood. In this presentation, we will focus on the interaction between the SEI and the underlying active electrode material. We would like to draw attention to the buried interface and emphasize its importance in both battery operation as well as photoelectron spectroscopy (PES) characterization of cycled electrodes.

We derived a model in which the buried interface between the bulk electrode material and SEI in cycled Li-ion battery electrodes is suggested to incorporate an electric potential gradient [1]. This model is based on PES results from different cycled electrode materials that all show relative binding energy shifts between the components of the surface layer and the active lithium-ion storage material depending on the state of lithiation. We were able to obtain this information for cycled battery electrodes by PES depth profiling using different photon energies. Our results therefore demonstrate that synchrotron PES depth profiling is a valuable tool to distinguish surface and bulk spectral contributions in battery electrodes which is crucial for consistent data interpretation.

References:
[1] J. Phys. Chem. Lett. 7, 1775 (2016).

S. McKeown Walker 07.12.16, 17:15

ARPES studies of the STO (001) 2DEG

S. McKeown Walker[1], Z. Wang[2], F.Y. Bruno[1], S. Ricco[1], A. Tamai[1], A. de la Torre[1], E. Golias[3], A. Varykhalov[3], D. Marchenko[3], P. Hlawenka[3], Y. Wang[4], Z. Ristic[5], N.C. Plumb[2], M. Shi[2], M. Hoesch[6], T.K. Kim[6], W. Meevasana[7], U. Diebold[8], J. Mesot[2,5], B. Moritz[4], M.S. Bahramy[9], P.D.C. King[10], T.P. Devereaux[4], M. Radovic[2], J. Sanchez-Barriga[3], F. Baumberger[1,2]

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9 RIKEN Center for Emergent Matter Science (CEMS), Japan
10 SUPA, School of Physics and Astronomy, University of St Andrews, UK

Two-dimensional electron gases (2DEGs) in $SrTiO_3$ arise in many configurations, for example at the $LaAlO_3/SrTiO_3$ interface and in $SrTiO_3$ based electric double layer transistors. The $LaAlO_3/SrTiO_3$ 2DEG in particular is a prominent system within the field of oxide electronics and spintronics. A detailed knowledge of the band structure of such 2DEGs aids the interpretation of their transport properties and plays an essential role in efforts to engineer novel behaviours in these systems. However interfaces in engineered heterostructures are inherently inaccessible to VUV-ARPES, a surface sensitive band structure probe. I will present ARPES measurements of the 2DEG discovered at the bare (001) surface of $SrTiO_3$, which is an accessible alternative for investigating the band structure of $SrTiO_3$ based 2DEGs. I will discuss the general electronic structure of this $SrTiO_3$ based 2DEG and describe the theoretically predicted Rashba spin-splitting which has eluded detection even, as I will show, by spin-resolved ARPES [1]. Finally I will present measurements that reveal the evolution of both the strength and nature of electron phonon interactions in the $SrTiO_3$ surface 2DEG as its carrier density is tuned [2].

References:
[1] Physical Review B, 93, 245143 (2016).
[2] Nature Materials, 15, 835 (2016).

M. Rahn 07.12.16, 17:30

All-in/all-out magnetic order in rare earth iridates

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5d transition metal oxides combine effects of strong spin-orbit coupling, electronic itinerancy and correlation on the same energy scale. In rare earth pyrochlore iridates ($R_2Ir_2O_7$) in particular, this complex situation leads to an unconventional insulating ground state, which cannot be understood in the usual Mott-Hubbard scenario. Furthermore, $R_2Ir_2O_7$ are also candidates for topologically non-trivial electronic states in the bulk (the Weyl semimetal). A key condition for the protection of the Weyl nodes is that the magnetic order must not break the cubic symmetry. This would be the case for the so-called all-in/all-out magnetic structure. I will be the reporting on a number of resonant x-ray scattering experiments that we have recently performed to investigate the magnetic ground state in these compounds.

Oxygen reduction reaction on graphene in Li-air batteries

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Oxygen reduction reaction (ORR) plays a key role in lithium-air batteries (LABs) that attract great attention thanks to their high theoretical specific energy several times exceeding that of lithium-ion batteries [1]. Because of their high surface area, high electric conductivity, and low specific weight, various carbons are often materials of choice for applications as the LAB cathode. Unfortunately, the possibility of practical application of such batteries is still under question as the sustainable operation of LABs with carbon cathodes is not demonstrated yet and the cyclability is quite poor, which is usually associated Li_2CO_3 byproduct formation [2]. It is generated at the cathode surface due to lithium superoxide (intermediate product) or peroxide (final discharge product) reactions with carbon [3,4]. However, the mechanisms of carbon reactivity toward these species are still unclear. Here, we report an *in situ* X-ray photoelectron spectroscopy study of oxygen reduction reaction on graphene electrode in Li-air battery. Although lithium peroxide (Li_2O_2) and lithium oxide (Li_2O) reactions with carbon are thermodynamically favorable, neither of them was found to react even at elevated temperatures. In contrast, superoxide species were demonstrated to be strongly reactive towards carbon. Using model chemical systems, we study reactivity of graphene with different concentration of vacancies and impurities towards lithium and potassium superoxides. As a result, we suggest detailed mechanism of carbon electrode degradation in LAB.

References:
[1] J. Phys. Chem. Lett. 1, 2193 (2010).
[2] Energy & Environmental Science 6, 750 (2013).
[3] ACS Nano 9, 320 (2015).
[4] Nano Letters 13, 4697 (2013).

Abstracts of the Key Note and Public Lecture at the Science Day

Thursday, 8th of December

Electronic Order in High-T_c Cuprate Superconductors

E. H. da Silva Neto[1]

1 University of California, Davis, United States

The study of the copper-oxide (cuprate) high-temperature superconductors provides a rich environment to study electronic orders and their interplay. In these cuprates, antiferromagnetism can be destabilized toward high-temperature superconductivity by either hole or electron doping. Besides these two phases, a periodic distribution of the electronic density, or charge order (CO), was recently detected in the Y-based cuprates [1], and echoed the long-known presence of stripe order in the La-based cuprates [2]. This additional electronic order found in the cuprates has been the focus of many cuprate studies over the last five years. In particular, this topic has benefited from advances in the resonant x-ray scattering (RXS) technique, which can access specific electronic states due to its element specificity. In this talk, I will review a series of RXS experiments that have advanced our understanding of the CO in the cuprates. First, I will discuss a combined scanning tunneling microscopy (STM) and resonant X ray scattering (RXS) experimental approach that established the universality of a CO competing with superconductivity in the holed-doped cuprates [3]. I will also present RXS measurements that demonstrated for the first time the presence of charge order in the electron-type cuprate NCCO [4]. A comprehensive study of CO in electron-doped cuprates as a function of doping, temperature, and magnetic fields, shows that CO does not require a pseudogap precursor state. We also find that while CO is universal to all cuprates, its relationship with superconductivity is not. Finally, open questions in the field, as well as prospects for future experiments, will also be discussed.

References:

[1] Science 337, 821 (2012).
[2] Nature 375, 561 (1995).
[3] Science 343, 393 (2014).
[4] Science 347, 282 (2015).
[5] Science Advances 2 (8), e1600782 (2016).

Solar Energy in an Emerging Country, Perspectives and the Need for International Cooperation

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Solar energy is like a dream in islands like Cuba where high irradiation levels are achieved. The Sun is an amazing and powerful source of energy but it needs also to be reached by other means. In this talk the perspectives of exploitation of solar for photovoltaics in Cuba will be addressed by following a human pathway. The history of Cuba, Havana University, Physics Faculty and the Solar Cells Laboratory will be also linked with international cooperation. This story will show how collaboration can make the difference, sometimes in term of just a single person. In summary, this conference expects to show the challenges and expectations of the PV community in Cuba and how collaboration plays a key role.

Abstracts of the Oral Presentations at the Science Day

Thursday, 8th of December

S. Kaskel 08.12.16, 10:40

In situ-observation of novel switching phenomena in highly porous Metal-Organic Frameworks

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2 Abteilung Probenumgebung, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

A unique phenomenon observed only in a limited number of materials is porosity switching in the crystalline solid state. Such flexibility was predicted 1998 for MOFs by Kitagawa and later termed "3rd Generation MOFs". Despite these early discoveries, among the about 20.000 coordination network structures only few compounds reveal substantial switching or breathing transitions or related stimuli responsive properties. Until today, the essential structural requirements for the construction of such bi- or multistable frameworks are unknown. One reason for this lack of knowledge is the difficulty in elucidating the complex structural changes induced by gases. In order to characterize the adsorbate-induced structural transformations, it is necessary to capture local and global structural information under variable, externally applied gas pressures in situ. The development of such in situ characterization techniques is essential (EXAFS, XRD, NMR, EPR) to monitor switching during adsorption/desorption cycling. A new phenomenon recently encountered by in situ methods is Negative Gas Adsorption (NGA). While the mechanism could be explained by the aid of theoretical DFT and GCMC calculations, yet the underlying principles to predict such a phenomenon in other MOFs are unknown. In any case, in situ XRD investigations are the key to investigate the structural transformations and get deep insights.
Only recently the tremendous potential of such switchable porous solids in energy storage, separation technologies, and sensing applications are brought to light.

H. Wadati 08.12.16, 11:00

Photoinduced demagnetization and insulator-to-metal transition in ferromagnetic insulating $BaFeO_3$ thin films

H. Wadati[1]

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We studied the electronic and magnetic dynamics of ferromagnetic insulating $BaFeO_3$ thin films by using pump-probe time-resolved resonant x-ray reflectivity at the Fe 2p edge. By changing the excitation density, we found two distinctly different types of demagnetization with a clear threshold behavior. We assigned the demagnetization change from slow (~150 ps) to fast (<70 ps) to a transition into a metallic state induced by laser excitation. These results provide a novel approach for locally tuning magnetic dynamics. In analogy to heat-assisted magnetic recording, metallization can locally tune the susceptibility for magnetic manipulation, allowing one to spatially encode magnetic information.

ARPES measurements of the ferroelectric bulk Rashba system GeTe

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GeTe has been predicted to provide Rashba split bulk bands around the band gap with a giant Rashba parameter up to 5 eVA. The fact that the spin direction is coupled to the ferroelectric polarisation of the material implies a ferroelectric switching of spin helicity.[1] Here, we firstly use conventional spin-polarized photoelectron spectroscopy (SARPES) to show that the surface states at the Fermi level show a strong Rashba splitting linked to the ferroelectric polarization.[2] Using a time-of flight spectrometer, we additionally revealed the spin texture of the bulk band again being in line with the externally determined ferroelectric polarization.[3]

References:
[1] Adv. Mater. 25, 509 (2013).
[2] Adv. Mater. 20, 516 (2016).
[3] arXiv:1512.01363.

J. Reichert 08.12.16, 11:40

Bisphenol A on Cu(111) and Ag(111): From Chemical Reactivity to Rotor Arrays

J. Reichert[1], S. Fischer[1], A. C. Papageorgiou[1], J. A. Lloyd[1], S. C. Oh, Ö. Sağlam[1], K. Diller[1], F. Allegretti[1], F. Klappenberger[1], A. P. Seitsonen[2], D. A. Duncan[1], M. Stöhr[3], R. J. Maurer[3], K. Reuter[3] and J. V. Barth[1]

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2 Physikalisch-Chemisches Institut der Universität Zürich, Switzerland
3 Theoretische Chemie, Technische Universität München, Germany

Bisphenol A is a common additive to everyday polymers and is in the spotlight due to its adverse health effects. Our investigations focus on its chemical and supramolecular behavior on solid metal surfaces employing scanning tunneling microscopy, synchrotron spectroscopy and dispersion-corrected density-functional tight-binding modeling. Our study reveals a remarkable sequence of thermally activated chemical transformations on Cu(111) and the emergence of a unimolecular network of rotors and stators on Ag(111). We propose molecular models stabilized by intermolecular hydrogen bonding and uncover the exact atomistic position of each molecule within the assembly as well as the driving force for the formation of the supramolecular rotors.

E. Vesselli 08.12.16, 12:00

Reverse Water–Gas Shift or Sabatier Methanation on Ni(110)? Stable Surface Species at Near-Ambient Pressure

E. Vesselli[1,2]

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The interaction of carbon oxides and hydrogen with the nickel (110) single crystal termination has been investigated up to 10^{-1} mbar *in situ* as a function of the surface temperature by means of infrared-visible sum frequency generation (IR–vis SFG) vibronic spectroscopy and by near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). Several stable surface species have been observed and identified. Besides atomic carbon and precursors for graphenic phases, nonequivalent CO species have been observed, evidencing the role of coadsorption effects, H-induced activation, and surface reconstruction. Carbonate and a metastable CO_2 species are detected, the latter being at the same time a precursor state toward dissociation into CO and O in the reverse water–gas shift (RWGS) process and a reactive species undergoing direct conversion in the Sabatier methanation. A picture is proposed, in which the two CO_2 conversion reactions proceed through parallel routes. Since also hydrogenation of CO is effective, an alternative and parallel CO_2 methanation mechanism involves RWGS, followed by the methanation of CO.

O. Daumke 08.12.16, 13:30

Structural studies of molecular machines

O. Daumke[1]

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Proteins of the dynamin family are mechano-chemical enzymes. They assemble in helical or ring-like polymers at cellular membranes and use the energy of GTP binding and hydrolysis to remodel the membrane. In this presentation, I will provide structural and functional insights into the assembly of selected members. In addition, I will show how the assembly process is regulated. Results of this work highlight the requirement of high resolution structural studies conducted at BESSY-II for the functional exploration of cellular processes.

Multi-MHz time-of-flight electronic bandstructure imaging of graphene on Ir(111)

H.-J. Elmers[1], C. Tusche[2], P. Goslawski[3], D. Kutnyakhov[1], M. Ellguth[1], K. Medjanik[1], S. Chernov[1], R. Wallauer[1], D. Engel[3], A. Jankowiak[3], G. Schönhense[1]

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3 Institut Beschleunigerphysik, Abteilung Betrieb Beschleuniger BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

In the quest for detailed spectroscopic insight into the electronic structure at solid surfaces in a large momentum range, we have developed an advanced experimental approach. It combines the 3D detection scheme of a time-of-flight momentum microscope with an optimized filling pattern of the BESSY II storage ring. Here, comprehensive data sets covering the full surface Brillouin zone have been used to study faint substrate-film hybridization effects in the electronic structure of graphene on Ir(111), revealed by a pronounced linear dichroism in angular distribution. The interference of directly emitted photoelectrons and electrons that have been scattered at the graphene layer cause darklines in the constant energy momentum patterns. These darklines originate from the quantum-mechanical transmission process of photoelectrons through the surface barrier and reveal previously hidden properties of the graphene layer. Time-of-flight momentum microscopy paves the way to 3D electronic bandmapping with unprecedented data recording efficiency.

Diffusion Pathways in Ion Conductors: Making the Most of Neutron-Diffraction Data

D. Wiedemann[1], M. Lerch[1]

1 Institut für Chemie – Festkörperchemie, Technische Universität Berlin, Germany

Sensors, electrolytes, energy storage systems: the fields of application for solid-state ion conductors are diverse. Scientific, as well as economic, interest in them is still on the rise. High-temperature neutron diffraction gives access to averaged positions of the atomic nuclei and their precise displacements, even when dealing with notoriously elusive chemical species like lithium ions. Notably, the high cost and ethical implications of such experiments, which are predominantly conducted at nuclear research reactors, demand the best possible evaluation.
If they are of adequate quality, data acquired from single-crystal or powder diffraction permit modeling of anharmonic thermally activated displacement. This enables the visualization of diffusion pathways and the determination of associated migration barriers *via* evaluation of probability-density function (PDF) and effective one-particle potential (OPP). But what about low-quality datasets or model failure? In these cases, an examination of the scattering-length density reconstructed *via* maximum-entropy methods (MEM) may at least yield semiquantitative results. As a supplement, heuristic means, or with difficult data, topological analyses are helpful. Within them, the framework of static species is searched for voids that are accessible for mobile ions. Representations of the procrystal-void surface provide quick insight into possible pathways, whereas Voronoi–Dirichlet partitioning (VDP) allows classifying them according to their suitability for certain ions.

A. Pietzsch 08.12.16, 14:30

Ground state potential energy surfaces around selected atoms from resonant inelastic x-ray scattering

A. Pietzsch[1], S. Schreck[1,§], S. Eckert[2], R. Jay[2], J. Niskanen[1], M. Fondell[1], P. S. Miedema[1], C. Såthe[3], S. Techert[456], V.N. Strocov[7], T. Schmitt[7], F. Hennies[3], J.-E. Rubensson[8], A. Föhlisch[1,2]

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3 MAX IV Laboratory, Lund, Sweden
4 FS-Structural Dynamics in (Bio)chemistry, Deutsches Elektronen-Synchrotron, Germany
5 Max Planck Institute for Biophysical Chemistry, Germany
6 Institute for X-ray Physics, Georg-August-Universität Göttingen, Germany
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§ Present address: Department of Physics, Stockholm University, Sweden

Thermally driven chemistry as well as materials' functionality are determined by the potential energy surface of a systems electronic ground state. This makes the potential energy surface a central and powerful concept in physics, chemistry and materials science. However, direct experimental access to the potential energy surface locally around atomic centers and to its long-range structure are lacking. Here we demonstrate how sub-natural linewidth resonant inelastic soft x-ray scattering at vibrational resolution is utilized to determine ground state potential energy surfaces locally and detect long-range changes of the potentials that are driven by local modifications. We show how the general concept is applicable not only to small isolated molecules such as O_2 but also to strongly interacting systems such as the hydrogen bond network in liquid water. The weak perturbation to the potential energy surface through hydrogen bonding is observed as a trend towards softening of the ground state potential around the coordinating atom [1].
The instrumental developments in high resolution resonant inelastic soft x-ray scattering are currently accelerating and will enable broad application of the presented approach. With this multidimensional potential energy surfaces that characterize collective phenomena such as (bio)molecular function or high-temperature superconductivity will become accessible in near future.

References:
[1] Nature Scientific Reports 6, 20054 (2016).

C. Roth 08.12.16, 14:50

Characterization of electrocatalysts using a combination of XAS and DRIFTS

C. Lentz[1], J. Melke[2], S. Jand[3], P. Kaghazchi[3], N. van der Bosch[4], U. Reinholz[5], H. Riesemeier[5], A. Guilherme Buzanich[5], M. Krishna Kayarkatte[4], I. Derr[4], A. Schökel[1,4], C. Roth[1]

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2 Institut für Anorganische und Analytische Chemie – Festkörperchemie, Albert-Ludwigs-Universität Freiburg, Germany
3 Institut für Chemie und Biochemie – Theoretische Elektrochemie, Freie Universität Berlin, Germany
4 Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany
5 Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

State-of-the-art catalyst for fuel cell applications are Pt nanoparticles supported on cheap and electron-conductive carbon. However, in the harsh conditions at the fuel cell cathode, carbon is not stable and catalyst degradation due to carbon support corrosion is a key issue in fuel cell technology. One concept towards enhanced durability is to replace carbon by more stable support materials, such as oxides. Substituting carbon by e.g. tin oxide can alter the catalytic activity significantly, as the catalytically active Pt nanoparticles interact with the support. We use CO as a probe molecule to study the particle-support interaction. A novel in-situ cell was developed to allow for a combination of X-ray absorption spectroscopy (XAS) and diffuse infrared Fourier transform reflectance spectroscopy (DRIFTS) at the same time and with high quality. The cell is based on a design of Drochner et al, in which a reference and the sample material are tested under identical conditions. Measurements with CO adsorbed on a Pt/SiO_2 (EuroPt-1) reference material and during continuous CO flow were recorded at different temperatures. Differences in IR spectra of CO adsorption on platinum nanoparticles can reveal information on the influence of the support as well as on the binding sites. In the study, XAS and DRIFTS were recorded simultaneously and analyzed with respect to kind of surface adsorbates, binding sites, coverage as well as nanoparticle structure. We benefit from the DRIFTS being able to distinguish between different CO binding sites (atop, bridge, analyzed also by DFT calculations) and XAS being able to probe adsorption (XANES) and nanoparticle structure (EXAFS).

Acknowledgment: BAMline @BESSY

Abstracts of the Young Scientist Session at the Neutron Day

Friday, 9th of December

Investigating the interphase formation on solid lithium ion conductors by neutron reflectometry

M. Weiß[1], B.-K. Seidlhofer[2], M. R. Busche[1], D. Schröder[1], M. Geiß[1], W. G. Zeier[1], M. Ballauff[2], and J. Janek[1]

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2 Institut Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

The discharging and charging of batteries require ion transfer across phase boundaries. In conventional lithium-ion batteries, Li+ ions have to cross the liquid electrolyte and only need to pass the electrode interfaces. Future high-energy batteries may need to work as hybrids, and so serially combine a liquid electrolyte and a solid electrolyte to suppress unwanted redox shuttles. This adds new interfaces that might significantly decrease the cycling-rate capability. Here we show that the interface between a typical fast-ion-conducting solid electrolyte and a conventional liquid electrolyte is chemically unstable and forms a resistive solid-liquid electrolyte interphase (SLEI). Insights into the kinetics of this new type of interphase are obtained by impedance studies of a two-chamber cell. The chemistry of the SLEI, its growth with time and the influence of water impurities are examined by state-of-the-art surface analysis and depth profiling [1].

Refrences:
[1] Nat. Chem. 8, 426 (2016).

S. Cabeza 09.12.16, 10:05

Load partition and damage characterization of cast $AlSi_{12}CuMgNi$ alloy with one- and two ceramic reinforcements

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2 Abteilung Mikrostruktur- und Eigenspannungsanalyse, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

The relationship between the microstructure of multiphase metal matrix composites and their damage mechanisms is studied. The matrix alloy $AlSi_{12}CuMgNi$ was combined with 15% vol. Al_2O_3 (short fibers), and with 7% vol. Al_2O_3 + 15% vol. SiC (short fibers and particles, respectively). The microstructure was characterized in 3D by means of synchrotron computed tomography at the BAMline (BESSY II, HZB). Neutron diffraction in-situ compression tests were performed at the E3 line (BERII, HZB) in order to reveal the load partition between the different phases. The damage occurrence could be discussed through the loss of load bearing capacity of some phases. Samples after compression were subjected to synchrotron CT to observe directly their damage. In total, the volume fraction of different phases, their distribution, their orientation, and the presence of defects and damage after compression were evaluated.
The influence on mechanical properties of adding one and two ceramic reinforcements was investigated. Phase-specific load partition analysis show damage in the Si phase, while Al_2O_3 short fibers carry the highest load without damage until failure. SiC load tendency evidenced minimal damage, which was related to partial de-bonding at its interface with the matrix. The evidence of damage observed by computed tomography confirmed the load partition analysis.

S. Krause 09.12.16, 10:20

Neutrons shed light on methane adsorption mechanism in a series of highly porous metal-organic frameworks

S. Krause[1], V. Bon[1], I. Senkovska[1], A. Franz[2], D. Wallacher[2], D.M. Többens[2], R.S. Pillai[3], G. Maurin[3], S. Kaskel[1]

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3 Institut Charles Gerhardt Montpellier, Université Montpellier, France

Metal-Organic Frameworks show the largest storage capacities for methane reported to date. Large pore sizes and functional sites on the inner surface can enhance the storage capacity, however the analysis of preferred adsorption sites remains a challenge for researchers. *In situ* neutron powder diffraction in parallel to methane adsorption has been carried out on DUT-49, the record holder in gravimetric methane storage (308 mg g-1 at 298 K, 110 bar). The location of methane in the pores could be refinement from the obtained diffraction patterns providing insight into the pore-filling mechanism. Besides fundamental understanding the study provides a base for improvement of future methane storage materials.

A. Gazizulina 09.12.16, 10:35

Study of the structure and magnetic interactions in dimer system $Ba_{(3-x)}Sr_xCr_2O_8$

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2 Abteilung Methoden zur Charakterisierung von Transportphänomenen in Energiematerialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

The spin dimer systems $Ba_3Cr_2O_8$ and $Sr_3Cr_2O_8$ are two candidates for the Bose Einstein condensation (BEC) of magnetic quasiparticles (triplons). We have recently reported on a peculiar non-linear tuning of the magnetic intradimer interaction constant J0 in the corresponding solid solution $Ba_{3-x}Sr_xCr_2O_8$ by varying the Sr content x. As the critical field Hc of the triplon BEC strongly depends on the magnetic interactions in the system, we have also probed the dependency of this critical field on x. Recently, we were able to grow single crystalline sample of $Ba_{2.9}Sr_{0.1}Cr_2O_8$ we have performed corresponding inelastic neutron scattering experiments to reveal the magnetic excitation spectrum.

Distribution of Sulfur in Carbon-Sulfur Nanocomposites Analyzed by Small-Angle Scattering Methods

S. Mascotto[1*], A. Petzold[2], G. Goerigk[2], D. Clemens[2], J. Scholz[1], A. Juhl[1], M. Fröba[1] and M. Ballauff[2]

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The analysis of the distribution of sulfur in nanoporous carbon hosts using small-angle scattering of x-ray and neutrons (SAXS and SANS) is here presented. Ordered porous CMK-8 carbon was used as host matrix and gradually filled with sulfur (20-50% wt.) via melt impregnation. Thanks to the match between the electron densities of carbon and sulfur, the porous nanocomposites present two-phase systems and the filling of the host material can be precisely followed by SAXS. The analysis using the Porod parameter and the chord-length distribution (CLD) approach determined the specific surface areas and the filling mechanism of sulfur, respectively. Moreover, using SANS the behavior of sulfur in the carbon matrix in the presence of a liquid phase, which might simulate the battery electrolyte, can be addressed. In the case of neutron scattering sulfur and carbon have different scattering length densities. The imbibition of the nanocomposites with liquids, which possess the same scattering contrast as carbon, enables the separation of the contribution of sulfur phase. Hence, valuable information on sulfur-carbon-solvent interactions can be gained. Thus, SAXS and SANS provide comprehensive characterization of the sulfur in porous carbon and valuable information for deeper understanding of cathode materials of lithium-sulfur batteries.

Abstracts of the HFM/EXED Session at the Neutron Day

Friday, 9th of December

O. Prokhnenko 09.12.16, 11:25

Current Status of HFM/EXED facility and its upgrade

O. Prokhnenko[1], P. Smeibidl[1], M. Bartkowiak[1], N. Stuesser[1], S. Kempfer[1], R. Wahle[1], S. Gerischer[1], O. Rivin[1], W-D. Stein[1], and B. Lake[1]

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The HFM/EXED facility offers users a unique combination of neutron scattering and strongest magnetic fields [1-2]. When operated at full current, High Field Magnet (HFM) generates continuous 26 T field which is available for neutron experiments at Extreme Environment Diffractometer (EXED). The latter is a time-of-flight instrument featuring diffraction and low-Q capabilities. In the last two years the instrument has being upgraded to enable inelastic neutron experiments [3]. In this talk the current status of HFM/EXED facility and its upgrade activities will be presented; a brief overview of the performed user experiments will be given. The procedures for planning experiments and applying for the beamtime will also be discussed.

References:
[1] IEEE Trans. Appl. Sup. 26, 4301606 (2016).
[2] Rev. Sci. Instr. 86, 033102 (2015).
[3] Nucl. Instr. Met. A 797, 121 (2015).

M. Pregelj 09.12.16, 11:45

Pursuit of spin nematicity in s=1/2 frustrated zigzag chain beta-$TeVO_4$

M. Pregelj[1], O. Zaharko[2], O. Prokhnenko[3], M. Bartkowiak[3], W. D. Stein[3], A. Zorko[1], D. Arčon[4], H. Berger[5]

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5 Ecole polytechnique fédérale de Lausanne, Switzerland

Nematic phases, where rotational symmetry of space is broken while the translational symmetries are kept, are found in many natural systems, e.g., liquid crystals. Yet, the question, if quantum magnets can also develop such an order, is still pending. In principle, spin-nematic states are considered as ordering of magnetic multipoles [1] and are thus extremely difficult to detect experimentally, since the latter do not interact with the magnetic field [1,2].
A lot of attention has been drawn by frustrated zigzag spin-1/2 chain model, where the ferromagnetic nearest-neighbor (NN) interaction J_1 competes with the antiferromagnetic next-nearest neighbor (NNN) interaction J_2. Here, the theory predicts that with the increasing magnetic field the vector-chiral ground state is followed by collinear spin-density-wave state and is close to the saturation succeeded by a spin-nematic (quadrupolar) phase [3]. Yet, $LiCuVO_4$ that is considered a model compound has a saturation field of ~45 T, which substantially narrows down applicable experimental techniques and thus precludes an undisputed experimental proof of the spin-nematic phase. Hence, new realizations of the J_1-J_2 chain model are highly desired.
Here we focus on beta-$TeVO_4$ that almost perfectly corroborates all theoretically predicted phase transitions [4,5], and thus offers another viewpoint on the zigzag spin-1/2 chain model. Moreover, more favorable exchange parameters (J_1/J_2 ~ -1.25 and J_2~30 K) lead to relatively low saturation field (B_{sat}~22 T) and thus allow for neutron scattering to be used for studying the spin-nematic phase that is predicted to develop above ~17 T. To establish the J_1-J_2 model and pursue the enigmatic spin-nematic phase, we thus performed single-crystal neutron diffraction experiment on EXED instrument using high-filed magnet at BER II at Helmholtz-Zentrum Berlin. I will present the obstacles we have faced, our approach to overcome them, the experimental results, and, finally, discuss possible explanations and outlook.

References:
[1] Phys. Rev. B 91, 174402 (2015).
[2] Introduction to Frustrated Magnetism (Springer-Verlag, Berlin, 2011).
[3] Phys. Rev. B 80,140402(R) (2009).
[4] Nat. Commun. 6, 7255 (2015).
[5] Phys. Rev. B 94, 081114(R) (2016).

K. Prokes 09.12.16, 12:05

Electronic properties of $U(Ru_{0.92}Rh_{0.08})_2Si_2$ in high magnetic fields

K. Prokes[1,2], T. Foerster[2], O. Rivin[3], M. Bartkoviak[3], S. Gerischer[4], R. Wahle[3], P. Smeibidl[3], O. Prokhnenko[3], Y.-K. Huang[5], A. de Visser[5] and J. Mydosh[6]

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5 University of Amsterdam, Amsterdam, The Netherlands
6 Kamerlingh Onnes Laboratory, Leiden University, The Netherlands

Heavy fermion systems remain in the focus of an intensive study. One of them is enigmatic superconducting URu_2Si_2 that orders below 17.5 K with yet unknown type of order, called therefore hidden. This material exhibits in fields between 35 and 38 T applied along the tetragonal axis several field-induced phases. These are, however, inaccessible with steady magnetic fields prohibiting neutron diffraction in stable thermodynamical conditions. Critical fields can be, however, shifted to accessible range by a suitable doping. For instance, doping few percents of Rh for Ru leads to a quick disappearance of the hidden order and superconductivity and a shift of the first critical field to values close to ~ 22 T. This enables a diffraction experiment using EXED-HFM facility. In this talk we report the high field electronic properties and the neutron diffraction experiment on the first high-field induced magnetic phase realized in a single crystal of $U(Ru_{0.92}Rh_{0.08})_2Si_2$. This phase appears at low temperatures in fields applied between 21 and 38 T and is built up from equal U moments of about 1.4 μ_B pointing along the c axis and arranged in an up-up-down configuration as one moves along the a axis. Our results, that include high-field magnetization and electrical transport results, suggest a significant Fermi surface topology modifications across metamagnetic transitions.

Field-dependent superconducting anisotropy and Pauli-paramagnetism in $YBa_2Cu_3O_7$ studied by time-of-flight small-angle neutron scattering from vortices in high fields

R. Riyat[1], E. Blackburn[1], E.M. Forgan[1], A.S. Cameron[2], A.T. Holmes[3], O. Prokhnenko[4], M. Bartkowiak[4], W.-D. Stein[4] and A. Erb[5]

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2 Institut für Festkörperphysik, Technische Universität Dresden, Germany
3 Science Directorate, European Spallation Source ERIC, Sweden
4 Abteilung Hochfeldmagnet, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
5 Crystal Growth, Walther-Meißner Institut für Tieftemperaturforschung der BAdW, Germany

We report on the evolution with magnetic field up to 25 T of the vortex lattice (VL) in fully-oxygenated $YBa_2Cu_3O_7$, studied by time-of-flight small-angle neutron scattering on the HFM-EXED beamline. The VL structure results indicate a de-pairing by field of the superconductivity along the crystallographic **b** (CuO chain) direction. Superconductivity along the chain direction is stronger at low field than that along **a**, but is weaker at high field. This change is indicated by the change of VL structure with field. The intensity of the diffracted signal gives the spatial variation of magnetisation caused by the VL. Surprisingly, this does not fall off rapidly with field, despite the de-pairing effect, and we ascribe this to Pauli-paramagnetism in the (de-paired) vortex cores. This adds a novel spin contribution to the standard "orbital" effect of supercurrents in the VL state, which is only observable in a superconductor for which the upper critical field in Tesla is larger than the critical temperature in Kelvin.

Abstracts of Poster Session – Science Day at BESSY II

Thursday, 8th of December

0 HZB CoreLabs - New Infrastructures for Current and Future Users

Wolter B, Seidlhofer B-K, Brandt A, Staier F, Vollmer A

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

0 X-Ray CoreLab: Various Methods for Material Research

Tovar M, Genzel C, Schorr S

The X-Ray CoreLab provides a variety of modern X-Ray diffraction methods. An outstanding feature is the in-situ analysis of structural phase transitions, the investigation of structure, microstructure and texture of thin layers, as well as the analysis of internal tensions in materials. The X-Ray CoreLab will serve co-workers of HZB as well as external academic and industrial partners.

0a Spinterface at a real-life copper surface of a potential molecular quantum bit based on the Blatter radical

Ciccullo F, Glaser M, Giangrisostomi E, Ovsyannikov, Casu MB

We demonstrate that a full-plastic derivative of the pyrene Blatter radical is a potential molecular quantum bit. The deposition of the pyrene Blatter radical on a CuBe surface, a simulation of industrial copper, reveals that the spinterface layer is different from the rest of the radical film, whereas its spin is maintained at the interface depending on the local nature of the CuBe surfaces.

0b Influence of the fluorination of CoPc on interfacial charge transfer

Balle D, Adler H, Grüninger P, Karstens R, Glaser M, Chassé T, Peisert H

The electronic structure of cobalt phthalocyanine (CoPc) and hexadecafluorophthalocyanine on Cu-inercalated graphene/Ni(111) is investigated by photoemission and X-ray absorption spectroscopy. It is found that the fluorination of the phthalocyanine affects considerably the charge transfer from the substrate to the central metal atom of the Pc.

0c Mn L-edge X-ray Absorption Spectroscopy on Photosystem II and prototypical Mn complexes in solution

Kubin M, Kern J, Chatterjee R, Gul S, Fuller FD, Kroll T, Guo M, Lundberg M, Odelius M, Löchel H, Quevedo W, Erko A, Föhlisch A, Bergmann U, Mitzner R, Yachandra VK, Yano J, Wernet Ph

Here we present and discuss our recent progress on Mn L-edge XAS of Photosystem II and multinuclear Mn compounds, structural mimics of the Mn_4CaO_5 cluster in PS II. The interpretation of the spectra in an ab-initio theoretical framework is outlined on the basis of complementary PFY-XAS spectra of mononuclear Mn-complexes. X-ray induced sample damage is addressed.

0d A Combined FT-IR and Soft-X-Ray Spectroscopic Approach on Aqueous Ammonium and Ammonia

Ekimova M, Quevedo W, Szyc L, Wernet P, Odelius M, Nibbering ETJ

We investigated the hydrogen bonding (HB) of ammonium and ammonia in aqueous solution using FT-IR and soft-x-ray spectroscopic methods. We present a novel liquid flatjet system with which solution phase soft-x-ray absorption spectroscopy can be performed. The experimental results compared with QM-MD calculations provide microscopic insight into the nature of HB of these small inorganic systems.

0e Soft x-ray beam damage of a solid Mn(III) complex determined with Mn L-edge absorption spectroscopy

Ludwig J, Kubin M, Ekimova M, Mitzner R, Weniger C, Föhlisch A, Kern J, Yachandra V, Nibbering E, Yano J, Wernet P

Soft x-rays are widely used for L-edge spectroscopy on transition-metal compounds, but also cause beam damage due to photoreduction. For acquiring damage-free data it is necessary to determine the acceptable threshold of x-ray dose for spectroscopy. Here we compare the dose dependent photoreduction in L-edge absorption spectra of Mn(III) with Mn(II) compounds and discuss the underlying mechanisms.

0f Magnetic properties of free metal-benzene complexes

Bülow C, Zamudio-Bayer V, Lindblad R, Timm M, Terasaki A, von Issendorff B, Lau JT

We investigate the mono and di-benzene complexes of Mn^+ and Cr^+ with XAS and XMCD in the gas phase to study the effect of 18- electron shell closure on the spin state. XAS and XMCD spectra show that 3d electrons in $CrBz^+$ and $MnBz^+$ are localized and therefore the clusters have a magnetic moment whereas in dibenzenes the electrons are delocalized and the 3d magnetic moment is quenched.

1c Tuning the flexibility in MOFs by SBU functionalization

Krause S, Bon V, Kavoosi N, Senkovska I, Müller P, Wallacher D, Többens DM, Mueller U, Kaskel S

A combination of powder XRD with gas adsorption experiments, performed at the KMC-2 beamline, has been used for monitoring of the guest-induced phase transitions in the series of flexible MOFs JLU-Liu-4(Zn). The strong correlation between the size of the monocarboxylic acid, coordinated to the metal cluster, and structural transition amplitude could be observed.

3 Interplay of magnetic coupling and anisotropy of $Ho_3N@C_{80}$ endohedral fullerenes on ferromagnetic substrates

Bernien M, Nickel F, Miguel J, Arruda LM, Kipgen L, Blümel N, Krüger D, Britton A, Schierle E, Weschke E, Kuch W

Ho^{3+} has a very high magnetic moment and strong magnetic anisotropy. In $Ho_3N@C_{80}$ three Ho ions are encapsulated in a fullerene cage and coupled together with a non-collinear alignment of their magnetic moments. By means of angle-dependent XAS and XMCD at T = 4.5 K and B = 6 T we find that the net moment of $Ho_3N@C_{80}$ couples ferromagnetically to Ni but antiferromagnetically to Co substrates.

4 Magnetism and structural changes in $Fe_{60}Al_{40}$ films under Ne^+ irradiation

Smekhova A, Szyjka Th, Eggert B, Cöster B, La Torre E, Walecki D, Salamon S, Ollefs K, Bali R, Lindner J, Rogalev A, Weschke E, Banerjee R, Sanyal B, Schmitz-Antoniak C, Wende H

XANES, EXAFS and XMCD techniques have been applied to probe substantial changes in Fe magnetic moments and the local environment in $Fe_{60}Al_{40}$ films along the order-disorder phase transition caused by Ne^+ irradiation of different fluences and energies. An increased magnetic polarization, drastic changes of coercivity, a rearrangement in the expanded unit cell and structural distortions were observed.

4a X-ray absorption study of thermally-induced electrocyclic ring closure of iron porphyrin molecules on Au(111)

Arruda LM, Ali MdE, Bernien M, Nickel F, Kopprasch J, Schierle E, Weschke E, Czekelius C, Oppeneer PM, Kuch W

Metalloporphyrins' stability and flexibility make them well-suited candidates for use in molecular spintronics. In this work we investigate iron octaethylporphyrin (FeOEP) and its transition to iron tetrabenzoporphyrin (FeTBP) through a ring-closure reaction on a Au(111) single crystal substrate. NEXAFS, XMCD, and DFT results are presented to display the modifications resulting from this process.

4b Thermal-, Light-, and X-ray-Induced Spin-State Switching of an Fe(II) Complex Adsorbed on a Graphite Surface, and its Tuning by Ligand Modification

Kipgen L, Naggert H, Bernien M, Nickel F, Arruda LM, Britton AJ, Ossinger S, Tuczek F, Kuch W

The control of the spin state of adsorbed molecules between high-spin state and low-spin state has been envisioned to provide building blocks for future miniaturized spintronic devices. We report the complete spin switching of an Fe(II) complex adsorbed on HOPG by temperature, light, and x rays. The addition of methyl groups to the parent molecule partially quenches the spin switching.

5 MAXYMUS at low temperatures

Stahl C, Ruoß S, Simmendinger J, Weigand M, Bechtel M, Schütz G, Albrecht J

The Scanning X-ray Microscope MAXYMUS has been upgraded with a low temperature cryostat based on liquid Helium to reach sample temperatures down to 20K. We present high spatial resolution low temperature magnetic x-ray images of the flux density distribution in the high-Tc superconductor YBCO obtained through XMCD measurements of a soft magnetic sensor layer (CoFeB).

6 Skyrmion Hall Effect Revealed by Direct Time-Resolved X-Ray Microscopy

Litzius K, Lemesh I, Krüger B, Bassirian P, Caretta L, Richter K, Büttner F, Sato K, Tretiakov OA, Förster J, Reeve RM, Weigand M, Bykova I, Stoll H, Schütz G, Geach GSD, Kläui M

Magnetic skyrmions are topologically stabilized nanoscale spin structures that show promise for future spintronic devices if they can be moved reliably. Employing scanning transmission x-ray microscopy, we report the pump-probe observation of reproducible skyrmion trajectories at room temperature in ultrathin multilayer films driven by spin orbit torques and we investigate the skyrmion Hall effect

7 Ptychographic Imaging of Magenetic Materials at MAXYMUS X-ray Microscope

Bykova Iu, Weigand M, Keskinbora K, Sanli U, Gräfe J, Bechtel M, Goering E, Stoll H, Baylan S, Richter G, Schütz G

Ptychography is an X-ray diffraction imaging technique, which achieve spatial resolution of few nanometers. However magnetic contrast imaging with diffraction techniques is still quite challenging because of low scattering on magnetically contrasted structures. We are going to show the first results of the implementation of ptychography at MAXYMUS microscope for magnetic contrast visualization.

8 Phase control in a pair of coupled magnetic vortex oscillators

Vogel M, Wild J, Schwarzhuber F, Zimmermann B, Zweck J, Back C

Magnetic Vortex Oscillators coupled via their stray fields are a possible building block for synchronization networks in a wide frequency regime. For information processing in such networks control over coupling between oscillators is crucial. Here we show that it is possible to control the phase relation between two oscillators by joule heating one of them.

11 Surface Composition of Free Nanoscale Aerosols Probed by X-ray Photoelectron Spectroscopy

Antonsson E, Raschpichler C, Langer B, Marchenko D, Rühl E

We study the local surface composition of mixed NaCl/Na_2SO_4 aerosols (d=100 nm) using photoelectron spectroscopy. The NaCl/Na_2SO_4 aerosols serve as model systems for salt aerosols, which are abundant in the atmosphere. The results indicate that surface enhancement of ions takes place and the results are interpreted using a model where the two salts do not co-crystallize.

14 Spin-polarized Current Induced Changes in $Ni_{80}Fe_{20}$ Half Ring Nanostructures

Khan MI, Cramm S, Nemšák S, Parlak U, Hackl J, Doğanay H, Gottlob G, Bürgler D, Schneider CM

The spin-polarized current induced changes in diamond patterns are investigated by time resolved X-ray PEEM. We observe the nucleation of diamond patterns in 1 µm wide $Ni_{80}Fe_{20}$ half ring structures due to the rise of temperature of rings by current pulses. Furthermore, we observe the elongation, propagation and also the transformation in diamond patterns due to the spin-torque effect.

15 On the reduction behavior of CeO_2 (100) and (111) surfaces

Hackl, Duchon, Müller, Mouls, Gottlob, Khan, Cramm, Nemšák, Schneider

Cerium oxide has an ability to store and release oxygen by changing its oxidation state between CeO_2 and Ce_2O_3. This gives ceria catalytic properties with many applications. Here CeO_2 islands with (100) and (111) oriented surfaces are grown in-situ and used as model catalysts. The chemical state of ceria islands during reduction in an H_2 ambient is observed with photoemission electron microscopy.

16 Study of magnetoelectric coupling of a thin layer of Fe deposited on a $BaTiO_3$ single crystal surface

Mouls C, Hackl J, Doganay H, Khan I, Cramm S, Cezar JC, Nemšák S, Schneider CM

Here we study the magnetoelectric coupling between a thin ferromagnetic Fe layer deposited on a ferroelectric $BaTiO_3$ substrate. Ferroelectric and ferromagnetic domains are observed with x-ray photoemission electron microscopy with respectively x-ray linear dichroism (XLD) contrast at the t2g orbitals of the L3 Ti edge and x-ray magnetic circular dichroism (XMCD) contrast at the Fe L3 edge.

25 In-system study of $SnCl_2$ precursor layers: First step towards the synthesis of Pb-free perovskites at EMIL

Felix R, Llobera-Vila N, Hartmann C, Klimm C, Wargulski DR, Hartig M, Wilks RG, Bär M

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 $SnCl_2$ 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.

26 MetVBadBugs - XRF and NAP-XPS characterization of drug uptake in multi-resistant bacteria

Dietrich P, Bahr S, Thissen A, Kjaervik M, Unger W, Streeck C, Beckhoff B

Multi-resistant bacteria embedded in infectious biofilms are one of the largest future threats in human healthcare. The mechanism of drug uptake and the origin of resistancy is quantitatively not well characterized and understood. Modern X-ray and synchrotron excited spectroscopic methods like XRF and NAP-XPS under ambient pressure conditions and liquid media will add new insights into this field.

28 Low Energy and Photo Electron Emission Microscopy at Near Ambient Pressure Conditions

Schaff O, Breitschaft M, Hagen S, Funnemann D, Thißen A, Fu Q

LEEM/PEEM allows to study dynamic processes at surfaces, like thin-film growth, surface reactions, and phase transitions at lateral and energy resolutions of below 5 nm and 250 meV, respectively. The technical capabilities of the SPECS PEEM P90 have been enhanced such, that operation under near ambient pressure conditions and even in operando is possible using synchrotron light for excitation.

31 Spin effects in graphene

Marchenko D, Varykhalov A, Sanchez-Barriga J, Rader O

The induced spin splitting of the graphene Dirac cone has the potential for numerous spintronics applications. In our work we experimentally show that the spin splitting of the graphene Dirac cone can be varied in a wide range of values, the spin texture can have spin-orbit- or exchange-type behavior, be in- or out-of-plane.

32 Interface formation of Titanium and Tantalum thin films onto $LiNbO_3$

Uwe V, Steffen O

We present results of detailed chemical interface analyses of sputtered Tantalum and Titanium thin films as potential adhesion and barrier layers onto cleaned piezoelectric substrate material $LiNbO_3$ with respect to their temporal stability up to 24 h and thermal stability up to 600°C in vacuum. The main technique for surface clean is a special Helium plasma, the analysis is done using AR-XPS.

34 Single bunch extraction by SAW driven bunch chopper

Vadilonga S, Zizak I, Petsiuk A, Erko A, Roshchupkin DV

Surface acoustic waves (SAWs) travel on the surface of solids, temporarily creating grating-like structures with amplitude up to one nanometer and near-sinusoidal deformation profile. Using electronically pulsed SAW synchronized with the arrival of the synchrotron X-ray pulses we successfully isolated the single bunch with a time resolution in the order of 100 ns.

35 Observation of sagittal diffraction of x-rays by surface acoustic waves in Bragg geometry

Vadilonga S, Zizak I, Petsiuk A, Erko A, Roshchupkin DV

X-ray Bragg diffraction in sagittal geometry on the Y cut of langasite crystal modulated by surface acoustic waves (SAWs) was studied at the BESSY II synchrotron radiation facility. This experiment shows that the propagation of the SAWs creates a dynamical diffraction grating on the crystal surface, and it can be used for space-time modulation of an X-ray beam.

37 MXCuBE2 - Next-generation experiment control for macromolecular crystallography experiments at the BESSY II photon source

Hellmig M, Kastner A, Weiss MS

The latest version of MXCuBE has been put into operation on both tunable HZB-MX beamlines. MXCuBE2 now integrates the interface to the automatic sample changer and the sample-centring functionality into the main control software which strongly improved the reliabiltiy of the beamline operation. Furthermore it provides the basis for the implementation of more complex data-collection protocols.

38 Facilities for Macromolecular Crystallography at the HZB

Gerlach M, Feiler C, Förster R, Gless C, Hellmig M, Huschmann F, Kastner A, Malecki P, Röwer K, Schmuckermaier L, Steffien M, Ühlein M, Wilk P, Weiss MS

The MX-group at the HZB operates three beamlines. With more than 400 PDB depositions in 2016, they are currently among the most productive MX-stations in Europe. They feature state-of-the-art experimental stations and ancillary facilities, serving 100 research groups across Europe. BL14.1-2 are equipped with Pilatus detectors and sample changer robots, providing a high degree of automation.

39 The expert MX data processing system XDSAPP

Röwer K, Weiss MS

XDSAPP is an expert user interface for the fast and automated processing of X-ray diffraction images from single crystals with XDS. Additional software like SFCHECK, Pointless, XDSSTAT and phenix.xtriage are used for automatic decision making. We present the latest developments and features of the program.

40 The SpectroLab for Macromolecular Crystallography

Hauß T, Gerlach M, Weiss MS

Next to the three beamlines for Macromolecular Crystallography (MX) the HZB-MX-group operates the SpectroLab. It is equipped with a micro-spectrophotometer which allows to measure the absorbance of tiny protein crystals in the UV-VIS spectral region.

41 Defining the landscape of EPHA2 Inhibition by Clinical Kinase Inhibitors

Kudlinzki D, Heinzlmeir S, Linhard V, Witt K, Saxena K, Lakshmi Gande S, Sreeramulu S, Médard G, Klaeger S, Qiao H, Helm D, Kuster B, Schwalbe H

The receptor tyrosine kinase EPHA2 has emerged as a therapeutic target due to its involvement in disorders of the cardiovascular and nervous system, cancer or pathogen infections. We identified 24 off-target inhibitors using Kinobead screening, elucidated their binding mode and categorized interacting residues according their localization, conservation and impact on drug target selection.

42 Antibiotics interactions with ovine and equine serum albumins

Talaj J, Sekula B, Bujacz A

Serum albumin (SA) transports a wide range of ligands in the blood, among them antibiotics. Crystal structures of ovine and equine SA in complexes with ampicillin, oxacillin and chlortetracycline were determined. Interactions of hydrolyzed and unhydrolized forms of beta-lactam antibiotics with SA have been observed. Research supported by grant 2013/11/B/ST5/02271 from the National Science Centre

43 Structural insides into substrate tunnels of bacterial lipoxygenase from Pseudomonas aeruginosa

Kalms J, Banthiya S, Galemou Yoga E, Kuhn H, Scheerer P

Lipoxygenases are non-heme iron enzymes catalyzing the dioxygenation of polyunsaturated fatty acids. The reaction specificity of these enzymes has been used as parameter for their classification. Lipoxygenase of Pseudomonas aeruginosa (PA) oxygenates the substrates arachidonic and linoleic acid. Two crystal structures of PA_LOX show an active site bound endogenous lipid ligand in a tunnel.

44 The fine-tuned machinery of oxygen-tolerant [NiFe] hydrogenase

Schmidt A, Kalms J, Frielingsdorf S, Lenz O, Heymann M, Cohen A, Kern J, Szczepek M, Scheerer P

Hydrogenases are fine-tuned machines catalyzing the interconversion of hydrogen. Several crystal structures of membrane-bound [NiFe]-hydrogenase of R. eutropha wildtype or with substitutions in different redox states reveal a fine-tuned interplay between several pathways. Since this machine is sensitive to X-rays, free-electron laser techniques have been used to gain new structural insights.

45 Structural Characterization of Fluorescence Optimized Bacterial Phytochromes as Optogenetic Tool

Sauthof L, Schmidt A, Szczepek M, Qureshi B, Stevens T, Fernandez Lopez M, Velazquez Escobar F, Michael N, Krauss N, Lamparter T, Hildebrandt P, Scheerer P

Phytochromes are photoreceptors which were found amongst others in bacteria. They allow in vivo deep tissue imaging and therefore they are used as a template in optogenetic engineering. We studied the far red-light absorbing bathy phytochrome Agrobacterium tumefaciens (Agp2) and a photoactivatable infrared fluorescence mutant of Agp2 (PAiR2).

46 Specificity of the Rhodopsin - Transducin interaction

Kwiatkowski D, Heyder N, Lê Công K, Tiemann J, Hildebrand PW, Sczcepek M, Scheerer P

GPCRs transmit extracellular signals to activate intracellular G Proteins. Upon activation GPCRs undergo a conformational change, which allows G Proteins to bind. Structures of rhodopsin bound to G protein derived peptides and Gs bound to the adreno receptor provided structural insight in this interaction. Our studies give new insight into the common recognition mechanism of G proteins by GPCRs.

47 Topological control of 3,4-connected frameworks based on the Cu2-paddle-wheel node: tbo or pto, and why?

Krause S, Müller P, Grünker R, Bon V, Pfeffermann M, Senkovska I, Weiss MS, Feng X, Kaskel S

The crystal structures of MOFs, namely DUT-63–64 and DUT-77–79, containing up to 90 % of disordered lattice solvent molecules in the pores, could be unambiguously determined using datasets collected on the MX BL14.3 beamline. The topology of the frameworks can be controlled either by addition of topology directing agents or by varying the conformational degree of freedom in the trigonal ligand.

48 Fragment-screening by X-ray crystallography at the HZB MX-Beam Lines at BESSY II

Huschmann FU, Förster R, Gerlach M, Heine A, Hellmig M, Klebe G, Linnik J, Malecki PH, Metz A, Radeva N, Schiebel J, Röwer K, Steffien M, Ühlein M, Wilk P, Mueller U, Weiss MS

Fragment screening is a widely spread approach to identify compounds, which are able to bind to protein targets. Typically, binding fragments are identified by a cascade of biophysical methods and then further analyzed structurally by X-ray crystallography. We have put this pre-screening cascade on the spot and found that X-ray crystallography should be used as the primary screening method.

49 Crystal structure of human interferon-gamma receptor 2

Kolenko P, Mikulecky P, Zahradnik J, Cerny J, Kolarova L, Pham PN, Dohnalek J, Schneider B

Human interferon-gamma receptor 2 (IFNgR2) is a cell-surface receptor that plays a critical role in immunity against infections. A crystal structure of IFNgR2 was solved at high resolution. We have identified putative binding sites for interferon-gamma and receptor 1, the natural ligands of IFNgR2. Support: MEYS CR (CZ.1.05/1.1.00/02.0109, LG14009), GA CTU (SGS16/246/OHK4/3T/14), RVO: 86652036.

50 Structural studies of cold adapted GH2 family beta-D-galactosidase

Rutkiewicz-Krotewicz M, Bujacz A

The recently solved structure of cold-adapted beta-DG from Arthrobacter sp. 32cB and previously determined one from Paracoccus 32d proved to be functional in a form of a dimer. This atypical oligomerization, since GH2 beta-DGs are usually tetramers or hexamers, may be a key feature responsible for its environmental adaptation.

51 Structure Analysis of Human Prolidase and Its Mutants Reveals Several Prolidase Deficiency Disease Mechanism Modes

Wilk P, Piwowarczyk R, Uehlein M, Dobbek H, Mueller U, Weiss MS

Prolidase deficiency is a rare recessive disorder characterized in humans by diminished prolidase activity and manifested by a wide range of severe clinical symptoms. Several mutations responsible for the loss or the reduction of prolidase activity were identified. Here we analyze structurally both wild-type enzyme as well as a series of pathological mutants providing better understanding of PD.

52 Balancing activity and resistance to organic solvents by modification of residues in the access tunnel.

Prudnikova T, Kuty M, Liskova V, Bednar D, Rezacova P, Koudelakova T, Sebestova E, Kuta Smatanova I, Brezovsky J, Chaloupkova R, Damborsky J

The DhaA variant with greatly enhanced stability and tolerance of organic solvents but reduced catalytic activity was created in the enzyme's access tunnel. Our results demonstrate that the delicate balance between activity and stability in enzymes can be effectively manipulated by fine-tuning the diameter and dynamics of their access tunnels.

53 Searching for novel compounds for prostate cancer therapy.

Malecki PH, Carter DM, Specker E, Przygoda J, Heinemann U, Gohlke U, Mueller U, Weiss MS

Changes in histone lysine methylation pattern have been observed in cancer cells. Two isoforms of histone lysine demethylases – KDM4A and C, members of Fe^{2+} and alpha-ketoglutarate-dependent KDM4 family, are known to stimulate growth of prostate cancer. KDM4A and D have been chosen as structural models for targeting active site by compounds, which may prove useful in a clinical setting.

54 Mechanism of partial agonism in AMPA-type glutamate receptors

Eibl C, Salazar H, Chebli M, Plested AJR

Partial agonists activate receptors weakly even when they occupy all available binding sites. Here the authors use X-ray crystallography, electrophysiology and crosslinking to show that partial agonists of the AMPA type glutamate receptor drive adoption of multiple inactive forms, accounting for their limited efficacy.

55 Structural characterization of a light-gated potassium channel

Saponaro M, Kerruth S, Lunelli M, Ehrenberg D, Heberle J, Kolbe M

Potassium channels play a pivotal role in many biological functions and are critically involved in a variety of diseases. Since the first potassium channel structure was solved in 1998, we have gained many important insights into their function. We employed photoswitchable ligands to induce conformational changes and capture the dynamics of a light-driven bacterial potassium channel.

56 X-ray Crystallographic Fragment Screening for the Development of New h17beta-HSD14 Inhibitors

Bertoletti N, Zara L, Metz A, Braun F, Heine A, Klebe G, Marchais-Oberwinkler S

Human 17beta-HSD14 is a recently characterized enzyme. We initiated a fragment-based lead discovery campaign by screening a 96 fragment library assembled considering the Rule of 3 as a guideline. Fragments capable of binding to a protein binding pocket can be used to explore the chemical space with respect to scaffold diversity. The small size of the fragments makes them suitable for optimization.

57 In operando study on MnO_x thin films during electro-catalytic water oxidation using soft x-ray absorption and emission spectroscopy

Shaker MN, Tesch MF, Bonke SA, Simonov A, Spiccia L, Aziz EF

We present an in situ study on electrodeposited MnOx films to observe changes of the electronic structure that occur during electro-catalytic water oxidation. X-ray absorption spectra were taken in operando for different applied potentials tracking the successive change of the Mn oxidation state. Resonant inelastic x-ray scattering reveals the potential induced changes of the MnO_x valence states.

58 Spin-resolved time-of-flight momentum microscope METIS

Kampen T, Wietstruk M, Hagen S, Schaff O, Tusche C, Schoenhense G, Oelsner A

METIS consists of a newly designed lens with full 2pi solid acceptance angle at highest angular, energy and lateral resolutions and as - time-of-flight setup - a drift tube and a time resolving 2D-delayline detector or imaging spin detector. It is the ideal tool for electronic structure studies on small samples or areas, whenever a pulsed source, like synchrotrons or lasers can be used.

58a Electronic structure of small iron oxide molecular frameworks and their precursors in aqueous solution

Seidel R, Pohl NM, Kabelitz A, Schulz K, Emmerling F, Krähnert R, Aziz EF, Winter B

We conducted systematic photoelectron-spectroscopy measurements from a liquid microjet to investigate the early stages of molecular frameworks of iron oxo complexes relevant in FeO_x nanoparticle formation in aqueous solutions. Different amounts of NaOH were added to a $FeCl_3$ precursor solution to alter the Fe/OH ratio to observe formation of molecular Fe-OH-complexes before precipitation occurs.

58b Electron-transfer-mediated decay in aqueous solution as a unique probe of ion pairing and structure

Pohl NM, Richter C, Seidel R, Lugovoy E, Winter B, Aziz EF, Hergenhahn U

Liquid-microjet X-ray photoelectron spectroscopy and electron-electron coincidence measurements are performed from Lithium salts in aqueous solution to search for an experimental signature of electron-transfer mediated decay (ETMD). Our calculations and first experiments show that the ETMD spectrum is sensitive to the local environment of the Li^+ cation and can be used as a measure of ion pairing.

59 Silicon Nanostructures based Hydrogen Generation

Schleusener A, Schulz M, Koyuda DA, Chuvenkova OA, Parinova EV, Dietzek B, Turishchev Yu, Sivakov V

Herein, we report the top-down formation of Si nanostructures with a sufficient large optical band gap to drive the photocatalytic H_2 production. The surface structure of SiNSs was studied using XANES and XPS methods. The photocatalytic performance using gas chromatography was investigated in a H_2O-EtOH mixture and irradiated with green and blue light.

60 Rapid surface oxidation of antimony telluride as evidence for a universal trend in the chemical reactivity of tetradymite topological in-sulators

Volykhov A, Sánchez-Barriga J, Sirotina A, Neudachina V, Frolov A, Gerber E, Kataev E, Senkovskiy B, Knop-Gericke A, Rader O, Yashina L

Based on the results of a series of photoemission studies combined with quantum chemical calculations, we report relatively fast surface oxidation of the least explored tetradymite-type topological insulator, Sb_2Te_3, under ambient conditions. The clean surface reacts rapidly with molecular oxygen and slowly with water, though humidity plays an important role at the stage of the oxide-layer growth.

61 A curious interplay in the films of N-heterocyclic carbene Pt(II) complexes upon deposition of alkali metals

Makarova A, Grachova E, Niedzialek D, Solomatina A, Sonntag S, Fedorov A, Vilkov O, Neudachina V, Laubschat C, Tunik S, Vyalikh D.

The newly discovered series of Pt(II) complexes reveals intriguing structures, topologies, and light emitting properties.This makes them attractive for biomedical, sensing and electronic applications.Herein, we report on the observation of curious physicochemical interactions between in situ produced polycrystalline supramolecular films of the Pt(II) complexes and deposited Li, Na, K and Cs atoms.

62 Intrinsic resolving power of XUV diffraction gratings measured with Fizeau interferometry

Manton J, Gleason S, Sheung J, Byrum T, Jensen C, Jiang L, Kaznatcheev K, Dvorak J, Jarrige I, Abbamonte P

We introduce a method for using Fizeau interferometry to measure the intrinsic resolving power of a diffraction grating. This method is more accurate than traditional techniques based on a long-trace profiler (LTP), since it is sensitive to long-distance phase errors not revealed by a d-spacing map. We demonstrate 50,400 resolving power for a mechanically ruled XUV grating from Inprentus, Inc.

63 Oxygen vacancies in Sr_2FeMoO_6 thin films

Saloaro M, Angervo I, Hoffmann M, Adeagbo WA, Granroth S, Palonen H, Huhtinen H, Majumdar S, Laukkanen P, Hergert W, Ernst A, Paturi P

Oxygen vacancies have been identified as a key factor for improving the properties of Sr_2FeMoO_6 thin films toward spintronic applications. Therefore, we have studied the effect of oxygen vacancies in post-annealed Sr_2FeMoO_6 films. The HAXPES (HIKE, KMC-1) and magnetic results will be supplemented with the theoretical calculations as well as Raman and positron annihilation spectroscopy results.

64 The temperature dependent electronic structure, magnetic interactions and photoinduced magnetization in $Pr_{0.6}Ca_{0.4}MnO_3$ thin films

Elovaara T, Granroth S, Tikkanen J, Majumdar S, Felix Duarte R, Huhtinen H, Paturi P

To gain further insight into the mechanisms behind the colossal magnetoresistive (CMR) behaviour of the perovskite manganite $Pr_{0.6}Ca_{0.4}MnO_3$, low-temperature HAXPES measurements and SQUID magnetometry have been performed on thin films of the material. In particular, we have focused on explaining the recently observed role of optical illumination in biasing and triggering the CMR transition.

65 Tuning surface plasmon resonance in Co/Ga-codoped ZnO nanowires

Käämbre T, Sutka A, Kooser K, Kook M, Kisand V, Pärna R, Felix Duarte R

Solvothermally synthesised optically transparent Ga/Co-codoped ZnO nanowires with strong surface plasmon resonance in the near-IR were studied by HiKE (at KMC-1) and seen to have rather uniform Ga levels throughout the wires, while traces of metallic Co in the bulk already at slightly above optimal content shed light on interplay of dopants and the origin of the optimisation limits.

66 Bulk carbonate active species in Ag_2O-Ag_2CO_3/Co_2FeO_4 nanoheterostructured magnetically separable photocatalyst: a HAXPES view

Käämbre T, Sutka A, Kooser K, Kook M, Kisand V, Felix Duarte R, Pärna R

A sizeable carbonate content in the bulk of Ag_2O/ferrite nanoheterostructures, which appears correlated with enhanced photocatalytic activity, is established from HAXPES measurements at KMC-1 beamline. The carbonate content, particularly that deeper in bulk, is seen to be depleted from sample (with decreased activity) recovered after several photocatalytic cycles.

66a Interface formation in SnS – based thin-film solar cells probed by hard x-ray photoelectron spectroscopy

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

The interface formed upon atomic layer deposition of ZnO or ZnO:N onto intentionally oxidized SnS is studied using HAXPES with different excitation energies. 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.

66b Impact of alkalis on the surface structure of Cu(In, Ga)Se_2 studied on in-system prepared model systems

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

Post-deposition treatments (PDT) of Cu(In,Ga)Se_2 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 at the HiKE endstation BESSY II KMC-1 to study model systems prepared in-system.

66c In-depth analysis of the Zn(O,S)/Cu(In,Ga)Se_2 interface formation

Kunze, Jackson, Hariskos, Siebert, Hartmann, Kozina, Felix, Gerlach, Yamashita, Ueda, Chikyow, Wilks, Witte, Bär

Solar cells based on Cu(In,Ga)Se_2 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_2 and Zn(O,S) respective thickness series have been studied. For a depth-dependent insight into the chemical interface structure excitation-energy dependent HAXPES measurements have been performed at BESSY II and SPring-8.

67 Thermodynamic Stability and Control of Oxygen Reactivity at Functional Oxide Interfaces: EuO on ITO

Gerber T, Lömker P, Zijlstra B, Besson C, Mueller DN, Zander W, Schubert J, Gorgoid M, Müller M

As a prototypical all-oxide heterostructure, the ferromagnetic insulator EuO is synthesized on conductive ITO substrates. HAXPES is employed to depth profile the chemical composition of the buried interface. We find that oxygen diffusion from ITO affects the EuO growth process. We present how to control the oxygen reactivity at the interface and discuss its origin in a thermodynamic analysis.

68 Thermally induced Ni^{2+} interdiffusion from NiO into Fe_3O_4 layers investigated by means of structural and x-ray spectroscopic techniques

Kuepper K, Kuschel O, Buß R, Spiess W, Schemme T, Wöllermann J, Balinski K, Kuschel T, N'Diaye AT, Wollschläger J

We investigated the evolution of the crystallographic, electronic, and magnetic properties of Fe_3O_4/NiO bilayers as result of thermally induced Ni-interdiffusion out of the NiO layer into the Fe_3O_4 thin film. For this purpose we employed HAXPES, accompanied by analysis of the structural and magnetic properties.

69 The chemical and electronic properties of inorganic lead-free $CsSnX_3$ perovskites

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

$CsSnX_3$ (X=Br, Cl, I) inorganic perovskites are promising Pb-free alternatives to the more common Pb halides. To identify the role of SnF_2 (addition of which during synthesis improves performance), halide composition, and deposition route, corresponding chemical solution- and vacuum-deposited $CsSnBr_3$ and $CsSnCl_3$ thin films, respectively have been characterized by HAXPES.

70 Structural properties of Al_2O_3/InAs(100) interfaces with and without pre-oxidized crystalline surfaces

Tuominen M, Mäkelä J, Dahl J, Yasir M, Granroth S, Kuzmin M, Laitinen M, Félix R, Polojärvi V, Tukiainen A, Lyytikäinen J, Punkkinen MPJ, Laukkanen P, Guina M, Kokko K

We have developed a proprietary oxide-deposition method to decrease the defect density at oxide/III-V interfaces. This technique improves the energy efficiency of III-V devices like photodetectors, transistors, solar cells, and LEDs. We present HAXPES depth profiling of Al_2O_3/InAs(100) interfaces that utilize the method to enlighten what kind of bonding environmental changes the technique induces.

71 Annealing-induced (optoelectronic) structure changes of In_2O_3 variants

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

In_2O_3 variants are highly transparent and conductive oxides with widespread applications. In our study, we systematically investigated the influence of annealing on the optoelectronic properties of intrinsic, Sn-doped, or H-doped In_2O_3 films by deliberate combination of x-ray diffraction, spectroscopic ellipsometry, Hall measurements, and synchrotron-based x-ray photoelectron spectroscopy.

72 NaF/KF post-deposition treatment of $Cu(In,Ga)Se_2$: Band gap widening due to formation of a K-In-Se surface species

Handick E, Reinhard R, Wilks RG, Bissig B, Kunze T, Alsmeier J-H, Köhler L, Krause S, Kreikemeyer-Lorenzo D, Weinhardt L, Blum M, Yang W, Gorgoi M, Ikenaga E, Gerlach D, Ueda S, Yamashita Y, Chikyow T, Heske C, Koch N, Buecheler S, Tiwari AN, Bär M

The performance of chalcopyrite-based thin film solar cells has recently been improved by performing alkali post-deposition treatments (PDT). We have used various x-ray spectroscopies to study the impact of different PDTs on the chemical and electronic absorber properties. After NaF/KF-PDT, we find significant band gap widening caused by the formation of a K-In-Se surface species.

73 Morphological Evolution of Li Electrodes in Li/Li symmetrical Cells and Li/Si half Cells: Studied by Synchrotron X-ray Tomography

Sun, Zielke, Markötter, Hilgér, Zhou, Moroni, Zengerle, Thiele, Banhart, Manke

Synchrotron X-ray tomography was employed to investigate the morphological evolution of electrochemically deposited or dissolved Li microstructures (LmSs, e.g. dendrites, fibers). A 3D characterization of electrochemically stripped Li electrodes with regard to electrochemically plated LmSs is presented. We clarify fundamentally the origin of the porous lithium interface growing into Li electrodes.

74 Optimizing visibility of phase gratings for Talbot-Lau X-ray imaging

Shashev Y, Kupsch A, Lange A, Britzke R, Bruno G, Müller B, Hentschel M

We investigated visibility of the phase grating upon variation of different parameters. Rotating around an axis parallel to the grid lines of the grating yields high visibilities for shorter propagation distances than for normal incidence case. Tilting the grating in scattering plane allows continuous tuning of grating's height that corresponds to an ideal phase shift for particular photon energy.

74a Analysis of Water Distribution in Gas Diffusion Layer Materials in a Point Injection Device by means of Synchrotron X-Ray Imaging

Ince U, Markötter H, George MG, Liu H, Lee J, Ge N, Bazylak A, Manke I, Banhart J

This study investigates water distribution in gas diffusion layer (GDL) materials used for polymer electrolyte membrane fuel cells based on ex-situ measurements with a point injection device. By synchrotron X-Ray imaging, water transport and distributions in various GDL samples are revealed according to the radial and angular displacements of water agglomerations relative to the injection point.

75 Time resolved WAXS studies on the crystallization of Al_{13} keggin clusters

Kabelitz A, Dinh AH, Emmerling F

We report on the in situ investigation of the Al_{13} sulfate synthesis by WAXS. Al_{13} sulfates were crystallized by precipitating hydrolyzed aluminum solutions by the addition of sodium sulfate. The measurements were performed using an acoustic levitator. The study provides information about the intermediates during the crystallization process.

76 In situ investigation of the mechanochemical formation of cocrystals using combined PXRD and Raman spectroscopy

Fischer F, Kulla H, Rademann K, Emmerling F

We present an in situ investigation of the mechanochemical formation of cocrystals using synchrotron XRD and Raman spectroscopy. This combination allows to study milling processes on the level of the molecular and crystalline structure thus obtaining reliable data for mechanistic studies. Thereby, mechanochemical syntheses can be optimized to isolate new crystal structures.

77 In situ investigation of mechanochemical syntheses of metal phosphonates

Akhmetova I, Wilke M, Emmerling F, Rademann K

We report on the in situ investigation of mechanochemical syntheses of metal phosphonates. The metal phosphonates are formed in milling reactions starting from a metal acetate and a phosphonic acid. The conversions are observed by synchrotron PXRD and Raman spectroscopy to shed light on the reaction mechanisms including possible intermediates.

78 Characterization of bioinspired and biological mineral materials using small and wide angle X-ray scattering

Wagermaier W, Gjardy A, Li C, Schmidt I, Seidt B, Siegel S, Fratzl P

Combining microbeam scanning SAXS/WAXS together with XRF or RAMAN at the BESSY II µSpot beamline allows the characterization of structure and composition of (i) the osteocyte network of bone, (ii) changes in polymer-metalfluoride particle composites during in-situ tensile testing and of (iii) bioinspired crystal calcium carbonate microlens arrays.

83 Optical and electronic properties of 1-adamantanethiol-aluminium hybrid clusters.

Knecht A, Bischoff T, Merli A, Möller T, Lau T, v. Issendorff B, Röhr M, Mitric R, Rander T

Plasmons, collective oscillations of delocalized electrons in metals, can be used for efficient energy transfer, resulting in fluorescence enhancement of dyes. Therefore, the radiative transition of a molecule (dye) needs to be in resonance with the absorption frequency of the plasmon. Here, we present a diamondoid-aluminium cluster hybrid system, designed to investigate these enhancement effects.

84 Absorption of diamondoid-metal hybrid systems studied with ion yield spectroscopy

Bischoff T, Knecht A, Merli A, Zamudio-Bayer V, Lau T, Möller T, Rander T

We investigate the possibility of combining diamondoids, UV luminescent carbon nanostructures that can be perfectly size and shape selected, and metallic particles on a sub-nm size scale to hybrid systems with tailored optical properties. Here, we studied the absorption of hybrids consisting of small thiolized diamondoids and cationic gold and silver clusters using ion yield spectroscopy.

88 Growth observations of Ga_2O_3 on various sapphire orientations as studied by synchrotron-based x-ray diffraction

Cheng Z, Hanke M, Vogt P, Bierwagen O, Trampert A

Ga_2O_3 was deposited on c- and a-plane oriented sapphire with molecular beam epitaxy and probed by ex-situ and in-situ synchrotron based XRD. This study determined the Ga_2O_3 phase transition thickness of about 3.3nm on c-plane sapphire. A 14.3 nm single phase alpha Ga_2O_3 was observed on a-plane sapphire. As shown in the strain relief dynamics, the alpha-Ga_2O_3 almost fully relaxed in the first 3nm.

89 Angle resolved photoemission spectroscopy (ARPES) on Tellurium single crystal

Titze F, Mulazzi M, Nazarzadehmoafi M, Janowitz C

We present the first ARPES data for Tellurium taken at the HU 5m-NIM and UE112-PGM-2a-1^2 beamline. While measuring the full electronic structure, the valence band maximum at the H-point is of special interest since recent calculations predicted a Weyl node there. We also show that more bands than predicted by bulk calculations are present at H-point, thus indicating the presence of surface states

90 Electronic structure of a single crystal $BiVO_4$ photocatalyst measured by angle-resolved photoemission spectroscopy

Mohamed M, May M, Kanis M, Janowitz C, Uecker RM, Brützman M, van de Krol R, Mulazzi M

We measured the valence band dispersion of $BiVO_4$, a promising photoanode material for solar water splitting, reaching an efficiency of 5% in a $BiVO_4$/a-Si tandem cell. The bands are flat, dispersing perpendicular to the (010) axis only. A non-dispersive peak in the gap was found and attributed to Mo point defects, whose consequences on the fundamental band gap size and character are discuss.

90a Evaluation of Residual Stress State of Additive Manufactured IN718 parts by means of synchrotron and neutron diffraction

Cabeza S, Mishurova T, Kromm A, Nadammal N, Klaus M, Genzel C, Wympory R, Boin M

Surface stress components from X-rays and synchrotron show high tensile values, with gradients along width and length of the sample. In the bulk of the material lower residual stresses are found, where the transversal component stays constant and near zero and the normal component is compressive.

90b Annihilation of structural defects in chalcogenide absorber films for high-efficiency solar cells

Mainz R, Simsek Sanli E, Stange H, Azulay D, Brunken S, Greiner D, Hajaj S, Heinemann MD, Kaufmann CA, Klaus M, Ramasse QM, Rodriguez-Alvarez H, Weber A, Balberg I, Millo O, van Aken PA, Abou-Ras D

In thin-film solar cells, structural defects may enhance electron-hole recombination and lower the efficiency. Cu-poor $Cu(In,Ga)Se_2$ films deposited at low temperature suffer from a high density of - partially electronically active - planar defects. Synchrotron-based in-situ X-ray diffraction reveals that these faults are rapidly annihilated when the film turns Cu-rich.

90c Surface residual stress analysis of SLM Ti-6Al-4V parts

Mishurova T, Cabeza S, Artzt K, Requena G, Haubrich J, Bruno G

Surface residual stresses in additive manufactured SLM parts were analysed for different fabrication parameters. As build samples present high tensile stress values on the surface, which increase significantly after release from base plate. Heat treated samples were totally relaxed. It is also proven that high laser energy density leads to the decrease of residual stresses.

99 The role of Re on ethylene epoxidation over Ag

Klyushin A, Carbonio E, Jones T, Hävecker M, Frei E, Lamoth M, Willinger E, Knop-Gericke A, Schlögl R

Shortly after the discovery of the first catalytic processes, it was realized that catalyst performance can be enhanced by adding very small concentrations of additional elements; known as promoters. In the present work, we study the promotion effect of Re on Ag catalysts in the ethylene epoxidation. The Ag-Re catalysts were synthesized by impregnation, co-precipitation and dipping methods.

100 Bridging the “pressure gap” in photo-electron spectroscopy: Chemical energy conversion related processes

Velasco Vélez JJ, Hävecker M, Pfeifer V, Wang R, Centeno A, Stotz E, Hofmann S, Skorupska K, Teschner D, Schlögl R, Knop-Gericke A

The discrepancy between high operation pressures applied in catalysis/electrocatalysis and low pressures during X-ray characterization is known in the community as the “pressure gap”. We will presents our actual advances in the investigation of solid-liquid and solid gas interfaces with PES in energy conversion related processes at environmental pressures.

102c Exploring the Ion Pairing Sensitivity of Electron Transfer Mediated Decay in Aqueous Lithium Solutions

Pohl MN, Richter C, Lugovoy E, Seidel R, Aziz EF, Abel B, Winter B, Hergenhahn U

The local structure of ions, e.g. in an aqueous solution of some salt, is still a topic of debate. We use solvated LiCl in a liquid jet as a prototype system, and focus on the formation of ion pairs (Li^+, Cl^-). We have recorded decay spectra (ETMD) after Li 1s ionization by an e^-,e^- coincidence method and show, that their shape can be sensitive to the participation of Li^+ in ion pairing.

103 The electronic structure of Tb silicide nanowires on Si(hhk) – From 2D to 1D

Appelfeller S, Franz M, Freter L, Jirschik H-F, Große J, Diemer Z, Hassenstein C, Schulze C, Füllert V, Prohl C, Döhring J, Dähne M

Monolayer high Tb silicide nanowires were grown by self-organisation on various vicinal Si(111) surfaces. Their electronic properties were analysed by ARPES and XPS, enabling a comparison with prior studies on Tb silicide monolayer films on planar Si(111) and on Tb silicide nanowires on Si(001). Electronic confinement effects are correlated with their structural dimensions derived by STM.

104 Synchrotron PEEM studies of MOCVD tin oxide covering the MAWCE silicon nanowires surface

Turishchev SYu, Schleusener A, Parinova EV, Chuvenkova OA, Koyuda DA, Marchenko DE, Ovsyannikov R, Tarasov AV, Sivakov V

Si nanowires massives (Metal Assisted Wet Chemical Etching Technology) were covered by MOCVD SnO_2. Developed surface composition and electronic structure were studied microscopically by synchrotron PEEM. Wires surface are inseparably covered by the layer of tin dioxide with metallic tin atoms inclusions and noticeable amount of oxygen vacancies formed sub-zone in structure`s surface band gap.

105 Photochromism on a Surface: Switching of Spiropyran on Bismuth

Nickel F, Bernien M, Kraffert K, Krüger D, Arruda LM, Kipgen L, Kuch W

Photochromic isomerization of molecules in direct contact with solid surfaces is important for the development of molecular electronics. Reversible light-induced switching between the ring-open and ring-closed configuration of a spiropyran derivative on the Bi(111) surface is presented, studied by NEXAFS, and compared to DFT simulations.

106 In-situ investigations on the norbornadiene/quadricyclane energy storage system on Pt(111) by UPS and HR-XPS

Bauer U, Bachmann P, Späth F, Düll F, Papp C, Steinrück H-P

Strained organic molecules, e.g. quadricyclane (QC) and its counterpart norbornadiene (NBD) are candidates for an energy storage system. We investigated the adsorption of QC and its conversion to NBD on Pt(111). We observe the conversion of QC to NBD below 120 K. HR-XPS reveals the decomposition of NBD at higher temperatures.

106a Temperature programmed high-resolution X-ray photoelectron spectroscopy of formic acid on Ni(111) and Pt(111)

Bachmann P, Bauer U, Späth F, Düll F, Papp C, Steinrück H-P

Formic acid has favorable properties as hydrogen carrier. We studied the adsorption at 130 K and temperature-dependent hydrogen release of formic acid on Ni(111) and Pt(111) using HR-XPS. Differences in the decomposition behavior, such as different desorption temperatures and the formation of CO on Ni(111) in contrast to the Pt(111) surface are revealed.

106b Polarization spectroscopy on graphene/metal interfaces

Jansing C, Mertins H-C, Gilbert M, Krivenkov M, Rader O, Gaupp A, Sokolov A, Wahab H, Timmers H

We present polarization measurements and the related x-ray natural linear dichroism at the C 1s edge of graphene on Co and Ni from which the strength of the bonding between graphene pi-states and metal 3d-states is deduced. Graphene on metals as Ni or Co shows a strong interaction with the substrate while graphene on Ni intercalated with Au shows a clear reduction in this bonding process.

106c Photoelectron elastic scattering probed by angle resolved X-ray photoemission from free SiO_2 nanoparticles

Langer B, Antonsson E, Halfpap I, Gottwald J, Rühl E

We report on X-ray photoelectron angular distributions from free SiO_2 nanoparticles after soft X-ray ionization above the Si 2p and O 1s absorption edges. The photoelectron angular anisotropy is found to be lower for photoemission from SiO_2 nanoparticles than the theoretical values for isolated Si and O atoms which is explained by elastic scattering of the outgoing electrons at neighboring atoms.

107 Magnetic phase identification of nanoparticles naturally produced in immune cells

Spasova M, Elsukova A, Zheng M, Salikhov R, Farle M, Frede A, Westendorf A, Luo C, Ryll H, Radu F, Wiedwald U

A subpopulation of splenic macrophages shows an enormous amount of endogenous, self-produced iron containing nanoparticles with a strong magnetic response, incompatible with the antiferromagnetism of natural ferritin usually found in macrophages. We investigate this magnetism by XAS/XMCD spectroscopy and elucidate the nature of the magnetic nanoparticles produced in immune cells.

108 Resonant Elastic X-ray Scattering (REXS) from the helical phase in Cu_2OSeO_3 at VEKMAG

Luo C, Poellath S, Schoen M, Radu F, Ryll H, Back C

We report successful resonant elastic x-ray scattering (REXS) experiments at VEKMAG. In the helical phase of the chiral magnet Cu_2OSeO_3 additional diffraction peaks appear around the (001) Bragg peak of the Cu L3 edge energy, caused by the modulated spin structure. Thus, reciprocal space maps are obtained utilizing a pin-hole diode.

109 XMCD measurements of $IrMn_3$ thin films

Taylor J, Luo C, Poellath S, Schoen M, Radu F, Ryll H, Back C

We report on high precision x-ray cicular dichroism (XMCD) measurments of thin film $IrMn_3$ non-colinear antiferromagnet at the VEKMAG endstation oft the PM2 beamline at BESSY 2. Antiferromagnetic behavior is observed in field dependent XMCD measurements on the Mn L3 edge, demonstrating the high XMCD resolution capabilities of the PM2 beamline.

113 PEAXIS: The new endstation for RIXS and XPS measurements at BESSY II

Schulz Ch, Hofmann T, Lieutenant K, Xiao J, Yablonskikh M, Habicht, Aziz EF

We present a new endstation for Photo Electron Analysis and X-ray resonant Inelastic Spectroscopy (PEAXIS) at BESSY II. After successful installation, beamline and endstation are currently in commissioning. The expected performance is outlined. Potential applications, for instance element-specific and momentum-resolved studies on thermoelectrics and catalysts for energy conversion, are discussed.

114 The new PGM beamline for HZB X-ray microscopy at BESSY II

Guttmann P, Werner S, Siewert F, Sokolov A, Schmidt J-S, Mast M, Brzhezinskaya M, Jung C, Follath R, Schneider G

We present here the setup of a newly designed beamline, results of metrology measurements of the new optical elements installed in the beamline, and also the first at wavelength measurements. This beamline will enable faster data acquisition together with an extension into the tender X-ray range to have access to two new important absorption edges, namely sulfur and phosphorus.

115 Upgrade of TOF spectrometer NEAT at Helmholtz Zentrum Berlin – first results

Russina M, Günther G, Drescher L, Schlegel M-C, Sucha V, Gainov R, Kaulich T, Graf W, Tsapatsaris N, Rolfs K, Mezei F, Urbahn B, Hellhammer R, Buchert G, Kutz H, Rossa L, Sauer O-P, Fromme M, Daske A, Grotjahn K

TOF spectrometer NEAT is best suited to study dynamic in abroad time domain. NEAT underwent recently a major upgrade and is currently in commissioning phase. The advanced features include novel integrated guide-chopper system several times more efficient as world leader IN5 at ILL. Substantial increase of the detector angle coverage was achieved by using He position sensitive detectors.

116 Small angle neutron scattering study of PAMAM dendrimers in aqueous solutions at different temperatures

Li T, Jafta C, Cheng Y

The solution structure of generation 4-6 PAMAM dendrimers were investigated by using small angle neutron scattering technique. The experiments were carried out on V4 instrument at HZB. The results indicated some intramolecular structure change upon varying the temperature.

117 Making the Most of Neutron-Diffraction Data: Lithium Diffusion Pathways in Ramsdellite-Like $Li_2Ti_3O_7$

Wiedemann D, Franz A

$Li_2Ti_3O_7$ is a fast and strongly anisotropic Li^+ conductor, whose diffusion pathways had not been studied in depth. We have conducted variable-temperature neutron diffraction to evaluate the results with maximum-entropy methods (MEM) and topological analyses. Interstitial migration along ribbons was identified as the major, framework migration through vacancies as the most probable minor mechanism.

118 Materials Characterization using Synchrotron Radiation Capabilities of the ICDD PDF-4 Databases

Blanton T, Fawcett T, Blanton J, Kabekkodu S, Papoular R

ICDD has developed tools for the analysis of synchrotron diffraction data. References in the Powder Diffraction File PDF-4+ can be converted to synchrotron diffraction patterns through the use of pattern simulations. Raw data patterns can be imported and analyzed for phase composition and quantity, and 270,000+ PDF entries with atomic coordinates can be imported into Rietveld refinement programs.

119 UNIFIT 2017 - the new spectrum processing, analysis and presentation software for XPS, AES and XAS

Hesse R, Denecke R

Now photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray ab-sorption spectra (XAS) can be analysed. The identification of the Auger lines is supported by new implemented data banks. The quantification can be carried out using integral or differential Auger spectra. In order to load and analyse SAM measurements or XPS mappings of more than 65536 spectra (265x256).

153 The complete upgrade of the experimental endstation of BESSY-MX BL14.2

Feiler C, Förster R, Gerlach M, Hellmig M, Kastner A, Müller U, Steffien M, Weiss M

Modern macromolecular crystallography requests high-throughput data collection without compromising on data quality. The experimental endstation of BL14.2 was completely upgraded. Comprising a unique nanodiffractometer, a Pilatus detector in conjunction with a G-ROB sample changer for fast sample mounting, it started its user operation recently with results confirming its superior performance.

154 Crystallographic Study on Endohedral Metallofullerene-based Single Molecule Magnets

Spree, Liu, Popov

Single-molecule magnets (SMMs) exhibit properties characteristic of bulk magnetic materials, but on a molecular level. Endohedral metallofullerenes (EMFs) encapsulating lanthanide metals ($DySc_2N@C_{80}$, $Dy_2ScN@C_{80}$, $Dy_2TiC@C_{80}$) have been proved as SMMs. In this project, we determined the structures of all the crystals we grew, using synchrotron radiation X-ray diffraction.

155 Investigation of erythropoietin interaction with serum albumin

Frydrysiak J, Bujacz A, Bujacz G

Human erythropoietin (EPO) is a 165 amino acid glycoprotein mainly produced in the kidney that promotes the production of red blood cells and a widely used drug in its recombinant form. Recent studies have shown that the complex creation between albumin and erythropoietin may prolong its therapeutic effects.

156 Structural insights into the activation mechanism of dynamin-like EHD proteins

Melo AA, Shah C, Hegde BG, Lundmark R, Langen R, Daumke O

EHDs are dynamin related proteins involved in membrane trafficking. The amino terminus of EHD2 regulates membrane recruitment and oligomerization and molecular details of the activation mechanism have remained obscure. Our study reveals mechanistic insights into the activation mechanism of the EHD as model for the dynamin superfamily.

157 Thermodynamic and crystallographic Charakterisation of preorganized Thrombin Ligands

Sandner A, Steinmetzer T, Heine A, Klebe G

Thrombin belongs to the group of chymotrypsin like serine proteases. It is involved in the blood coagulation. Most available thrombin inhibitors have drawbacks, such as a high bleeding risk and no available antidote or undesired interactions with other drugs or food ingredients. We characterized five ligands by xRay and ITC to estimate whether the new types of ligands experience less deficiencies.

158 Structural Analysis of Immune Response Regulator ZC3H12C and Cognate RNA element.

Garg A, Takeuchi O, Heinemann U

We present 1.9Å resolution structure of an endoribonuclease, ZC3H12C which plays crucial role in fine tuning of immune responses by targeting 3' UTR of immune response factors. We also present 1.3Å resolution structure of ZC3H12C cognate RNA, which adopt an unusual double helical conformation with 4x C.A and 2x G.U wobble base pairs.

159 Sequence to high-resolution structure: A minimal Photosystem II PsbO variant

Bommer M, Bondar N, Oschkinat H, Zouni H, Dobbek H, Dau H

PsbO is a beta barrel protein thought to facilitate rapid proton transfer away from the PSII reaction centre. Neutron diffraction may yield a first, static proton map. We present a workflow from an on-paper design of a stable core protein, via oligonucleotide gene synthesis, determination of an initial X-ray structure to growing millimetre crystals, maybe an initial neutron diffraction image.

160 Binding and turnover of halogenated phenols by reductive dehalogenase

Bommer M, Kunze C, Hagen WR, Uksa M, Schubert T, Diekert G, Dobbek H

Reductive dehalogenase removes halide substituents from often toxic organohalide pollutants. We have used X-ray diffraction on enzyme-substrate complexes to elucidate the routes of substrate turnover and the basis for selectivity. Photoreduction by the X-ray beam was partially able to drive the reaction.

172 In-operando imaging of media transport in electrode materials

Markötter H, Arlt T, Hilger A, Kardjilov N, Manke I

Understanding media transport in the porous materials of electrodes is a key issue in the development of energy materials, like e.g. for energy storage, electrolysis, fuel cells or batteries. This poster provides a brief overview on recent applications on this arising research field.

172a Visualizing Discharge Products in Sodium-Oxygen Battery Cathodes

Schröder D, Bender CL, Osenberg M, Hilger A, Manke I, Janek J

Synchrotron X-ray tomography was applied to elucidate the spatial distribution of discharge product (NaO_2) in the carbon cathode of sodium-oxygen batteries. We observe a particle density gradient along the cathode that scales with the current density applied. Our findings imply how the cathode in sodium-oxygen batteries can be better utilized for future applications.

172b In-operando synchrotron imaging of electrode materials in fuel cells

Markötter H, Haußmann J, Klages M, Seidenberger K, Wilhelm F, Arlt T, Scholta J, Manke I, Banhart J

The water distribution and evolution in a PEM fuel cell was studied via synchrotron imaging. The method development towards fuel cell research is presented in this poster. Water quantification and the identification of liquid water transport paths were conducted using radiography and tomography.

172c Characterizing damage evolution in metal-matrix-composites with x-ray refraction topography and in-situ tensile loading

Laquai R, Müller BR, Nellesen J, Kupsch A

In this study a metal-matrix-composite of aluminum matrix reinforced with alumina particles was investigated with x-ray refraction topography and in-situ tensile loading. It could be observed that after reaching a certain load the specific surface increased steadily. However, the classical radiographs taken for comparison show no damage in the sample.

173 In-operando Synchrotron X-Ray and Neutron Radiography Studies of Polymer Electrolyte Membrane Water Electrolyzers

Hoeh MA, Arlt T, Kardjilov N, Manke I, Banhart J, Fritz DL, Ehlert J, Lüke W, Müller M, Lehnert W

Investigate gas removal in porous transport layer and flow channel in Polymer Electrolyte Membrane (PEM) water electrolysis. Understand two-phase flow through the porous transport layer. Identify most efficient porous structures. Evaluate cost-reduction potential of alternative porous structures based on two-phase flow properties.

174 In situ and operando Tracking of Microstructure Degradation of Silicon Anode using Synchrotron X-ray Imaging

Dong K, Markötter H, Sun F, Manke I, Hilger A, Kardjilov N, Banhart J

The internal morphology and structure changes of silicon electrodes during cycling were revealed by in situ and in operando synchrotron radiography techniques.

175 Investigation of rechargeable Zn-MnO2 batteries with X-ray tomography

Osenberg M, Dimitrova I, Hilger A, Kardjilov N, Arlt T, Markötter H, Manke I, Banhart J

We present in-operando X-ray tomographic investigations of the charge and discharge behaviour of rechargeable Zn-MnO2 batteries. Changes in the three-dimensional structure of the zinc anode and the MnO2 cathode material after several charge/discharge cycles were analysed. Results are compared to the behaviour of a conventional primary cell that was also charged and discharged several times.

176 Investigation of two-phase flow in porous structures in PEM water electrolysers

Boraha D, Panchenko O, Hoeh M, Arlt T, Mahnke I, Bahnart J, Müller M, Lehnert W

The porous structures in a PEM water electrolyser play an important role. To optimize the performance of electrolysers an understanding of the gas evolution process and gas-water transport is essential. Gas evolution is modelled using a simplified approach and, another approach is suggested as future work. Flow behaviour is also visualized experimentally.

176a Virtual access to hidden texts - Study of ancient papyri

Arlt T, Lindow N, Baum D, Hilger A, Manke I, Hege H-C, Lepper V, Siopi T, Mahnke H-E

In the Papyrus Collection of the Egyptian Museum in Berlin like in other museums, a multitude of papyri is stored: fragments of different sizes and conditions of preservation. To get access to this source of profound knowledge about our cultural origin we have to reveal the texts hidden in these objects. We will report on first results on mockups of modern papyrus and fragments of ancient papyri, blank and written with Fe gall and carbon ink.

176b Synchrotron X-ray and neutron imaging for DMFC research

Arlt T, Wippermann K, Schröder A, Markötter H, Kardjilov N, Hilger A, Tötzke C, Banhart J, Manke I

Fuel cells are expected to contribute to a sustainable energy supply in future. Direct-methanol fuel cells are promising candidates for several mobile applications. Catalyst layers and gas diffusion layers are objects of current energy research at the Helmholtz-Zentrum Berlin. Complimentary ex-situ and in-operando experiments have been performed at the experimental stations CONRAD 2 and BAMline.

177 Surface response after atomic hydrogen treatment on common industrial high-density polyethylene (HDPE)

Schlebrowski T, Fischer CB, Wehner S, Yang C, Nefedov A

The interaction of atomic hydrogen and polymers is not completely understood, although it occurs during the most techniques used for e.g. carbon depositions on polymers. For a complete description it is inescapable to study these hydrogen processes, since sample interactions could occur. Our contribution shows first results of the surface response of HDPE with atomic hydrogen.

178 Deposition of nm sized a-C:H layers on common polyoxymethylene (POM)

Rösken LM, Catena A, Wehner S, Fischer CB, Yang C, Nefedov A

Amorphous carbon layers (a-C:H) have been deposited via plasma technique on industrial polyoxymethylene copolymer with increasing thicknesses to refine and improve surface characteristics. Synchrotron radiation contributes to understand the occurring processes between these unequal materials. SEM and AFM are used to analyze the specific topographies of the carbon coatings.

179 Grafting [Fe(III)(salten)] Complexes to Gold by Click Reactions: A Surface-Spectroscopic Study

Schlimm A, Tuczek F

Starting from a SAM of 1-azido-11-undecanethiolate on Au(111), we perform a click reaction with two ethynyltolyl-functionalized [Fe(III)(salten)] complexes. Before and after the click reaction the respective functionalized surfaces are investigated with the help of infrared reflection absorption spectroscopy (IRRAS), supported by X ray photoelectron spectroscopy (XPS).

180 Adsorption and orientation of large organic molecules on MgO/Ag(100)

Pechmann S, Fink RH

We investigated growth and orientation of large organic molecules with extended pi-systems on epitaxial MgO/Ag(100). As organic compounds alpha,omega-disubstituted quaterthiophene with two hexyl endgroups, as well as octaethylporphyrin and its metalated equivalent cobalt (II) octaethylporphyrin were studied with focus on NEXAFS dichroism as they exhibit long range ordered self-assembled monolayers

180a NEXAFS and XPS analysis of functionalized graphene surfaces for bio applications

Donskyi IS, Lippitz A, Haag R, Unger WES

Graphene prepared from Graphene oxide (GO) is used as a platform for functional 2D nanomaterials with diverse applications ranging from biosensors to antimicrobial surfaces. C and N K-edge NEXAFS and XPS spectroscopies at BESSY's HE-SGM beamline have been used to prove and control covalent functionalization of graphenic materials at ambient conditions for the synthesis of functional 2D-surfaces.

181 Quantitative Chemical Depth-Profiling by Synchrotron-Radiation-XPS: Developing a Valid Methodology for the Application to Core-Shell Nanoparticles

Hermanns A, Lippitz A, Radnik J, Unger WES

Synchrotron-radiation enables the adjustment of the XPS information depth and, thus, the visualization of depth profiles of the elemental composition within the first 10 nm of a surface. This project deals with the analysis of core-shell nanoparticles. It constitutes first steps towards a valid methodology for studying the surface chemistry of nanoparticles in a quantitative and accurate manner.

182 Nuclease activity of copper(II)-phenanthroline-complexes immobilized on silicon nitride films

Lange N, Dietrich PM, Gründler A, Lippitz A, Kulak N, Unger WES

Copper(II)phenanthroline complexes intercalate into DNA and induce DNA cleavage. Here, we investigate the nuclease activity of copper(II)phenanthroline complexes on silicon nitride films. 1,10-phenanthroline-5-carboxylic acid is immobilized at Si-NHx bonds via amide coupling followed by the formation of copper(II)phenanthroline complexes. XPS and NEXAFS were carried out at the HE-SGM beamline.

183 Structural Control and Hetero-Adduct Formation in Molecular Donor/Acceptor Pairs studied by NEXAFS Spectroscopy

Breuer T, Karthäuser A, Witte G

C1s-NEXAFS spectroscopy, AFM and XRD was used to study the structure of the molecular donor acceptor pairs PEN/C60 and PEN/PFP. For PEN/PFP molecular orientation and polymorphism can be controlled by inheriting the orientation of bottom to the top layer compound. For C60/PEN a hetero-adduct formation via Diels-Alder reaction is identified which also affects the subsequent film growth.

184 Investigation of active sites of polymer derived Fe-N/C catalysts for efficient oxygen reduction (ORR)

Melke J, Elsaesser P, Pardo L, Gerke F, Dreiser J, Nefedov A, Fischer A

ORR efficient Fe-N/C electrocatalyst can be synthesized by the pyrolysis of Fe/polymer precursor materials. For a further optimization of the materials the structure of the active sides and their formation needs to be investigated. In order to determine the structure of the active sides we measured the near edge x-ray absorption fine structure at the C, N K-edge and the Fe L2,3-edge.

184a Plasma synthesis of carbon based nanomaterials (CBNs)

Pattyn C, Berndt J, Strunskus T, Lecas T, Boulmer-Leborgne C, Hussain S, Canizares A, Ammar MR, Simon P, Dias A, Tatarova E, Raitses Y, Nefedov A, Kovacevic, E

We present results on the CBNs synthesized in plasmas from different types of carbon precursors. CBNs obtained in the plasma systems range from nanoparticles, nanotubes, nanowalls, nanorods to free standing graphene sheets. XPS and angle resolved NEXAFS analysis of CBNs was performed at HE-SGM station. The XPS and NEXAFS results are compared with those from ex- and in-situ Raman spectroscopy.

196a The Diffuse Scattering Pattern from Structured Surfaces

Soltwisch V, Fernandez Herrero A, Pflüger M, Probst J, Scholze F

Laterally periodic nanostructures were investigated with grazing incidence small angle X-ray scattering. To support an improved reconstruction of nanostructured surface geometries, we investigated the origin of the contributions to the diffuse scattering pattern which is correlated to the surface roughness.

196b Ageing of organic photovoltaic (OPV) PTB7-thin films by quantified synchrotron radiation investigated by photoelectron spectroscopy

Darlatt E, Muhsin B, Rösch R, Kolbe M, Gottwald A, Roth F, Hoppe H, Richter M

OPVs represent an alternative to inorganic solar cells. One disadvantage of organics in OPVs is their low stability against radiation. The study of ageing processes is therefore prerequisite for the fabrication of stable OPVs in the future. Our study presents a new irradiation protocol enabling the investigation of wavelength and photon amount dependent degradation effects in organic thin films.

196c Characterization of Sub-nanometer Cr/Sc Multilayer Systems for the Water Window

Haase A, Bajt S, Soltwisch V, Hönicke P, Scholze F

We report on the characterization of subnanometre Cr/Sc multilayers through the application of several analytical experiments. A combined analysis is shown and verified by Markov chain Monte Carlo sampling.

200 GISAXS on small sample volumes using large beams

Pflüger M, Soltwisch V, Probst J, Scholze F, Krumrey M

In Grazing Incidence Small-Angle X-Ray Scattering (GISAXS) experiments, the footprint of x-ray beams on the sample is significantly elongated. Traditionally, this has limited GISAXS measurements to long (> 10 mm) samples. We measured short (down to 4 µm) grating targets, both on empty substrates and surrounded by other nanostructures, opening GISAXS to new fields of application.

200a Characterization of nano-layers for transparent conductive oxides and power electronics by XRF and NEXAFS

Unterumsberger R, Streeck C, Pollakowski B, Rotella H, Nolot E, Beckhoff B

In the present work, transparent conducting oxide (TCO) layers and power electronics were analyzed using reference-free X-ray fluorescence (XRF) analysis to determine the absolute mass deposition of oxygen and aluminum and to reveal a possible change in the respective elemental depth profile due to annealing processes. Furthermore, the chemical binding state of these elements was analyzed as well.

200b Traceable chemical analyses of new liquid and solid battery components by X-ray spectrometry in UHV environment

Zech C, Graetz O, Raguzin I, Ivanov S, Müller M, Stamm M, Bund A, Börner M, Evertz M, Pyschik M, Nowak S, Grötzsch D, Malzer W, Beckhoff B

For a better understanding of the functionality of battery components we can determine the mass deposition and the oxidation state of elements on cathode and anode surfaces by reference-free X-ray fluorescence spectrometry and by X-ray absorption spectrometry, respectively. To characterize electrolyte solutions we use a fluid cell that enables soft X-ray investigations.

200c A compact and calibrateable von-Hamos X-Ray Spectrometer based on full-cylindrical HAPG mosaic crystals

Wansleben, Holfelder, Weser, Beckhoff

A high-resolution wavelength-dispersive spectrometer is realized by using up to 2 cylindrical HAPG crystals for a large solid angle of detection and hence high efficiencies. The energy range is 2.3-18 keV with an intended resolution of 2300. Its calibration involves detailed characterization of the optics and precise setup for traceable energy axis, response function and respective uncertainties.

200d A liquid cell for the analysis of biomolecules (e.g. proteins, chlorophyll) using soft X-ray excitation

Streeck C, Grötzsch D, Witte K, Dietrich P, Malzer W, Nutsch A, Stiel H, Unger W, Kanngießer B, Beckhoff B

For versatile applications, including vacuum instrumentation, a liquid cell was developed. Using ultra-thin windows, this cell enables X-ray absorption spectrometry in the soft X-ray range which is in particular interesting for the analysis of organic molecules in liquids or at the solid-liquid interface. NEXAFS of a protein at N K-edge and of chlorophyll a at Mg K-edge is demonstrated.

200e Characteristic diffuse scattering from rough lamellar gratings

Fernandez Herrero A, Soltwisch V, Pflüger M, Probst J , Scholze F.

We have studied the diffuse scattering contributions from lithographic manufactured nanostructures. Si-lamellar gratings with a well defined line edge roughness and line width roughness were investigated using EUV scatterometry. Each type of roughness leads to a resonant diffuse scattering pattern, showing the correlation between the type of roughness and the diffuse scattering contributions.

200f Recent determinations of X-ray fundamental parameters

Hönicke P, Kolbe M, Unterumsberger R, Pollakowski B, Beckhoff B

The development of new materials with distinct properties needs an analysis such as X-ray fluorescence analysis (XRF), which can provide independent information without any reference material. For a reliable quantitative XRF the atomic fundamental parameters involved are needed. Here, we present recent works on these parameters employing the calibrated instrumentation of the PTB.

200g Monodisperse nanoparticles with a polydisperse core: Separating the components using continuous contrast variation in SAXS

Garcia-Diez R, Gollwitzer C, Sarnacci K, Krumrey M

Continuous contrast variation in SAXS is a recent technique to characterize nanoparticles with an inner structure that is especially suited for polymeric nanoparticles. We applied this technique to core-shell particles with a PTFE core using fructose as contrast agent. By increasing fructose content and thus solvent density, a very narrow size distribution of the polymeric particles is observed.

CR Ultra-thin iron-silicate formation on Ru(0001)

Peschel G, Fuhrich AB, Klemm HW, Prieto M, Genuzio F, Menzel D, Schmidt Th, Freund HJ

The presented study addresses the growth and structure of ultra-thin iron-silicate films on Ru(0001). LEEM, LEED, XPS and XPEEM measurements are performed using the SMART microscope located at the UE49-PGM Beamline. Our studies reveal the formation of co-existing domains, having different structural characteristics as well as chemical composition. Finally we present a model for iron-silicate.

CR Silica Thin Films as Model System for Catalysis: A LEEM/PEEM study.

Prieto MJ, Klemm HW, Fuhrich A, Peschel G, Menzel D, Schmidt Th, Freund H-J

We will show results obtained with the SMART microscope, using in situ XPS, LEED and LEEM. For instance, in thick silica films a reaction front is observed during oxidation presumably due to evaporation of the topmost layers and oxygen intercalation. For the bilayer, no reaction front and XPS results show that the amount of oxygen intercalated can be controlled.

CR Alternative routes for magnetic data storage investigated by X-PEEM

Arora A, Ünal AA, Valencia S, Kronast F

The future data storage technologies require magnetization control to be ultrafast, robust and cost-effective. However, the conventional way of using magnetic fields for this is proving to be power consuming and inefficient for high density storage devices. Here we explore alternative routes to control magnetism by laser light or applied voltage using photo-emission electron microscopy with X-rays.

Abstracts of Poster Session - Neutron Day

Friday, 9th of December

1 Reconstruction of Greek Pottery and Provenance Studies of Greco-roman Coins Using Non-destructive Neutron

Siouris IM, Karkantonis T, Seira A, Balaska V, Katsavounis S, Hoser A

Neutrons are used to characterise archaic pottery and coins, from NE Greece. The aim is to supply data on the constituent minerals, firing and weathering conditions, the metallic phases, the corrosion products and uncommon additions deposited during burial.The results assisted to the restoration of the pottery and provided information on minting and provenance.

2 Neutron diffraction on the frustrated spin-1/2 chain linarite, $PbCuSO_4(OH)_2$, at low temperatures and high magnetic fields

Heinze L, Willenberg B, Hoffmann J-U, Wolter-Giraud AUB, Rule KC, Ouladdiaf B, Süllow S

An elastic neutron diffraction study on the frustrated spin-1/2 chain linarite, $PbCuSO_4(OH)_2$, is presented. Special emphasis was given on the high magnetic field and low temperature regime of the magnetic phase diagram for fields applied along the crystallographic b-axis. The magnetic moment evolution within the phase diagram was derived indicating that the phase transition IV-V is of first order.

3 Characterization of Residual Stress State by Neutron Diffraction and Residual Magnetic Field Mapping

Stegemann R, Cabeza S, Lyamkin V, Bruno G, Wimpory R, Boin M, Pittner A, Böcker A, Kreutzbruck M

Based on the residual stress characterization of tungsten inert gas welded S235JRC+C plates by means of neutron diffraction, the evaluation of residual stress with high spatial resolution GMR (giant magneto resistance) sensors is discussed. The experiments performed indicate an interdependence of residual stress changes and local residual magnetic stray fields.

4 Evaluation of Residual Stress State of Additive Manufactured IN718 parts by means of synchrotron and neutron diffraction

Cabeza S, Mishurova T, Kromm A, Nadammal N, Klaus M, Genzel C, Wympory R, Boin M

Surface stress components from X-rays and synchrotron show high tensile values, with gradients along width and length of the sample. In the bulk of the material lower residual stresses are found, where the transversal component stays constant and near zero and the normal component is compressive.

5 Antiferromagnetic structure in R_2Ni_2In (R = Er, Tm)

Baran S, Szytula A, Hoser A

The low temperature magnetic structure in R_2Ni_2In (R = Er, Tm) has been derived from neutron powder diffractometry data. The rare earth magnetic moments are parallel to the b-axis and form an antiferromagnetic structure related to the propagation vector k=[1/2,0,1/2]. In order to verify validity of obtained magnetic structure model a symmetry analysis was performed.

6 Magnetic ordering and magnetocaloric effect in the $NiMn_{1-x}Cr_xGe$ (0 <= x <= 0.25)

Szytula A, Baran S, Hoser A, Jaworska-Golab T, Marzec M, Dyakonov V

Magnetic ordering and magnetostructural properties of Cr-doped NiMnGe have been investigated. With increase of temperature a change of crystal structure from orthorhombic to hexagonal one is detected. A helicoidal magnetic order turns into ferromagnetic one with increase of Cr content. In temperature range close to critical temperature of magnetic order large magnetic entropy change is observed.

7 Crystal and magnetic structure of La-Sr-Mn-O solid solution doped with Ni

Sikolenko V, Karpinsky D, Efimov V, Troyanchuk I, Franz A, Schorr S

Neutron diffraction study of effects of substution Mn by Ni in complex manganese oxides are presented. It ishas been found, that a type of magnetic ordering changed from FM to AFM in a very narrow range of Ni doping. Possible explanations are discussed.

8 Crystal structure and magnetic exchange in (Sr, Sb)-doped lanthanum manganites

Efimov V, Karpinsky D, Troyanchuk IO, Sikolenko V, Frontzek M, Többens D

The crystal structure and magnetic properties of the compounds $La_{1-x}Sr_{2x}Mn_{1-x}Sb_xO_3$ with manganese ions in the 3+ oxidation state are studied. It is suggested that the observed ferromagnetism originates from the breakdown of orbital ordering and significant hybridization between the eg orbitals of Mn^{3+} and 2p orbitals of oxygen.

9 Analysis of the wide-angle X-ray (WAXS) and neutron (WANS) scattering data of non-graphitic carbons

Badaczewski FM, Pfaff T, Franz A, Loeh MO, Smarsly BM

We analyzed the microstructure of non-graphitic carbon samples by evaluating their WAXS and WANS patterns using the approach by Ruland and Smarsly to verify its applicability to WANS data. The WANS patterns of the carbon samples acquired show the expected reflexes and in addition some a strong SANS signal or a hydrogen background. The parameters obtained from both WAXS and WANS data agree well.

10 V2 -Cold Triple Axis Spectrometer with Multiple Energy Analysis Update

Lu Z, Hüsges Z, Meng, S, Quintero Castro D, Habicht K

Combined triple axis and high resolution spin-echo spectroscopies could be obtained by cold neutron 3-Axis spectrometer (FLEXX). A powerful MultiFLEXX option with large access region in wavevector and energy space has been updated and ready for external users to do overview measurements with little effort.

11 Upgrade of TOF spectrometer NEAT at Helmholtz Zentrum Berlin - first results

Russina M, Günther G, Drescher L, Schlegel M-C, Sucha V, Gainov R, Kaulich T, Graf W, Tsapatsaris N, Rolfs K, Mezei F, Urbahn B, Hellhammer R, Buchert G, Kutz H, Rossa L, Sauer OP, Fromme M, Daske A, Grotjahn K

TOF spectrometer NEAT is best suited to study dynamic in abroad time domain. NEAT underwent recently a major upgrade and is currently in commissioning phase. The advanced features include novel integrated guide-chopper system several times more efficient as world leader IN5 at ILL. Substantial increase of the detector angle coverage was achieved by using He position sensitive detectors.

12 In-situ Small Angle Neutron Scattering Characterization of Lithium Sulfur Batteries

Jafta CJ, Risse S, Yang Y, Clemens D, Petzold A, Goerigk G, Ballauff M

The lithium sulfur battery system is known for its complex chemical and electrochemical processes. One of these complexities is the precipitation process of sulfur and lithium sulfide at the end of charge and discharge. In an attempt to shed more light on this mechanism we present a novel electrochemical cell that allows for SANS characterization of an electrode in an operating cell.

13 Small angle neutron scattering study of PAMAM dendrimers in aqueous solutions at different temperatures

Li T, Jafta C, Cheng Y

The solution structure of generation 4-6 PAMAM dendrimers were investigated by using small angle neutron scattering technique. The experiments were carried out on V4 instrument at HZB. The results indicated some intramolecular structure change upon varying the temperature.

14 Polarizing neutron optics from HZB

Krist Th, Hoffmann J

Polarizing neutron optics is developed at HZB, like normal and radial benders and two-dimensional polarisation analysers for up to 5°, all showing polarisations around 95%. Also polarizing S-benders were built and tested with cross sections up to 60mm x 125mm for wavelength ranges down to 2 A. At a wavelength of 4.4A the maximum transmission was above 65% with a polarization above 98%.

15 Neutron optics developments

Krist Th, Hoffmann J, Schulz J

Neutron optical devices have been developed at HZB like solid state polarizing benders, collimators, cavities and 2D polarization analysers with polarizations up to 95% and polarizing S-benders showing polarization values up to 98%. A focusing silicon lens showed a gain of 5.6. Prism systems were shown to work as neutron energy analysers and focusing systems.

16 Interface Growth in FeCo-Si Multilayers determined with atomic resolution

Krist Th, Cho S-J, Hoffmann J

FeCo-Si multilayer are used as neutron polarisers. To optimise their performance, the thickness of interface layers should be reduced. Polarized neutron, x-ray reflectometry and in situ fast kinetic ellipsometry are used to characterize a model system of a monochromator with 5 bilayers. Using all these data it was possible to describe the growth of the multilayer system with atomic resolution.

17 In-Operando Characterization of PEMFCS Water Transport Using Neutron Radiography

Alrwashdeh SS, Manke I, Markötter H, Haußmann J, Kardjilov N, Klages M, Kermani MJ, Al-Falahat AM, Scholta J, Banhart J

We study a new type of flow field channel design for PEMFCs. Small barriers have been installed into the flow field channels in order to improve the supply of the catalyst with the reactant. Water distribution in the PEMFC studied with neutron imaging and compared the results with a reference cell. The new design water distribution is much more homogenous compared to the reference cell.

18 Neutron Imaging Applications

Kardjilov N, Manke I, Hilger A, Markötter H, Arlt T, Khanh TV, Al-Falahat AM, Banhart J

Neutron imaging has reached a new level after techniques based on contrast mechanisms alternative to the common beam attenuation have become available. In this way, properties of materials and complex systems can be resolved by position sensitive mapping exploiting diffraction, small-angle scattering and refraction signals.

19 Phase and Texture Evaluation in Dual-Phase Steel by Neutron Bragg-Edge Imaging

Tran VK, Woracek R, Penumadu D, Kardjilov N, Hilger A, Boin M, Markötter H, Tremsin A, Alrwashdeh SS, Al-Falahat AM, Manke I

The availability of suitable characterization techniques for polycrystalline materials is fundamental for the development of new materials, improving manufacturing processes and a better understanding of failure phenomena. The neutron based method "Bragg-edge tomography" is showcased for a TRIP steel that exhibits austenite to martensite transformation after tensile and torsional deformation.

20 First experimental tests of tensorial neutron tomography for quantitative measurements of magnetic vector fields

Hilger A, Kardjilov N, Manke I, Strobl M, Jericha E, Banhart J

Radiography and tomography with polarized neutrons allows for investigation of magnetic vector field distributions in 2D and 3D. We present quantitative 2D investigations and an approach for real 3D vector field (tensorial) tomography. Results from first experiments and from simulations are compared.

21 Various Prism Structures for Affecting Neutron Beams

Manicke T, Krist T

Sub millimetre prisms structures of silicon are used to achieve focusing, energy analysis or counteracting gravitational effects of neutrons in a lens, an energy analyser and a gravitation compensator. All three devices are realized and tested at two instruments at the BERII. We show simulations in Vitess and current measurement data.

22 Materials Characterization Unsing Neutron Radiation Capabilities of the ICDD PDF-4 Databases

Blanton T, Faber J, Blanton J, Kabekkodu S, Papoular R, Fawcett T

ICDD has developed tools for the analysis of neutron diffraction data. References in the Powder Diffraction File PDF-4+ can be converted to neutron CW or ToF diffraction patterns through the use of pattern simulations. Raw data patterns can be imported and analyzed for phase composition, and 270,000+ PDF entries with atomic coordinates can be imported into Rietveld refinement programs.

23 Intrinsic resolving power of XUV diffraction gratings measured with Fizeau interferometry

Manton J, Gleason S, Sheung J, Byrum T, Jensen C, Jiang L, Kaznatcheev K, Dvorak J, Jarrige I, Abbamonte P

We introduce a method for using Fizeau interferometry to measure the intrinsic resolving power of a diffraction grating. This method is more accurate than traditional techniques based on a long-trace profiler (LTP), since it is sensitive to long-distance phase errors not revealed by a d-spacing map. We demonstrate 50,400 resolving power for a mechanically ruled XUV grating from Inprentus, Inc.

24 Neutron Bragg-edge Imaging of Copper Samples with Different Heat Treatment Methods

Al-Falahat AM, Kardjilov N, Woracek R, Manke I, Markötter H, Boin M, Alrwashdeh S, Khanh T, Banhart J

Two different testing techniques based on neutron Bragg edge transmission imaging were carried out in order to resolve quantitatively the distribution of copper microstructure samples with a different heat treatment methods. Measurements of different copper samples revealing difference Bragg edge profile which are affected by their grain size.

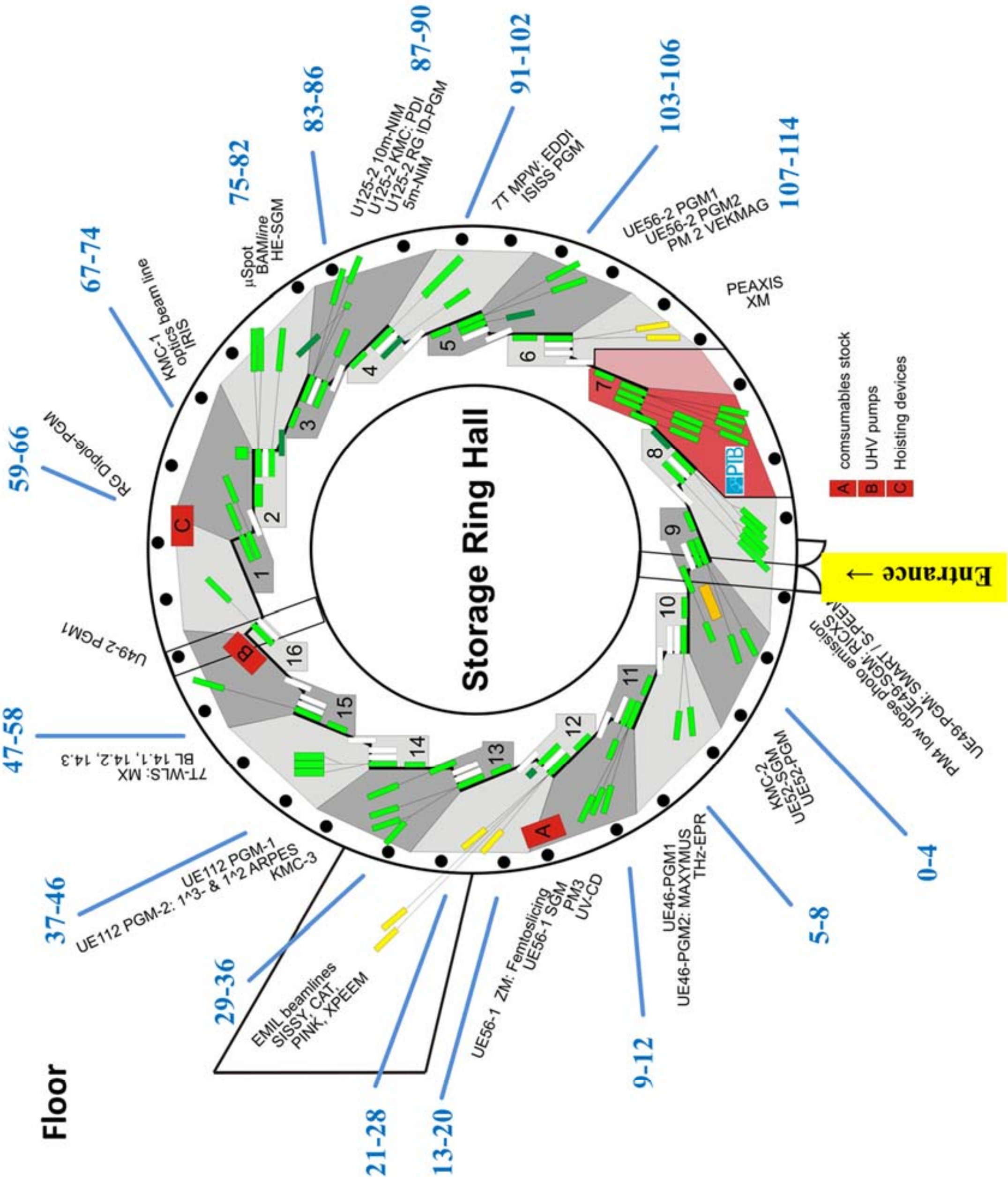
25 HZB CoreLabs - New Infrastructures for Current and Future Users

Wolter B, Seidlhofer B-K, Brandt A, Staier F, Vollmer A

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

Floorplan of Poster Session – Science Day at BESSY II

Thursday, 8th of December



Floorplan of Poster Session – Science Day at BESSY II

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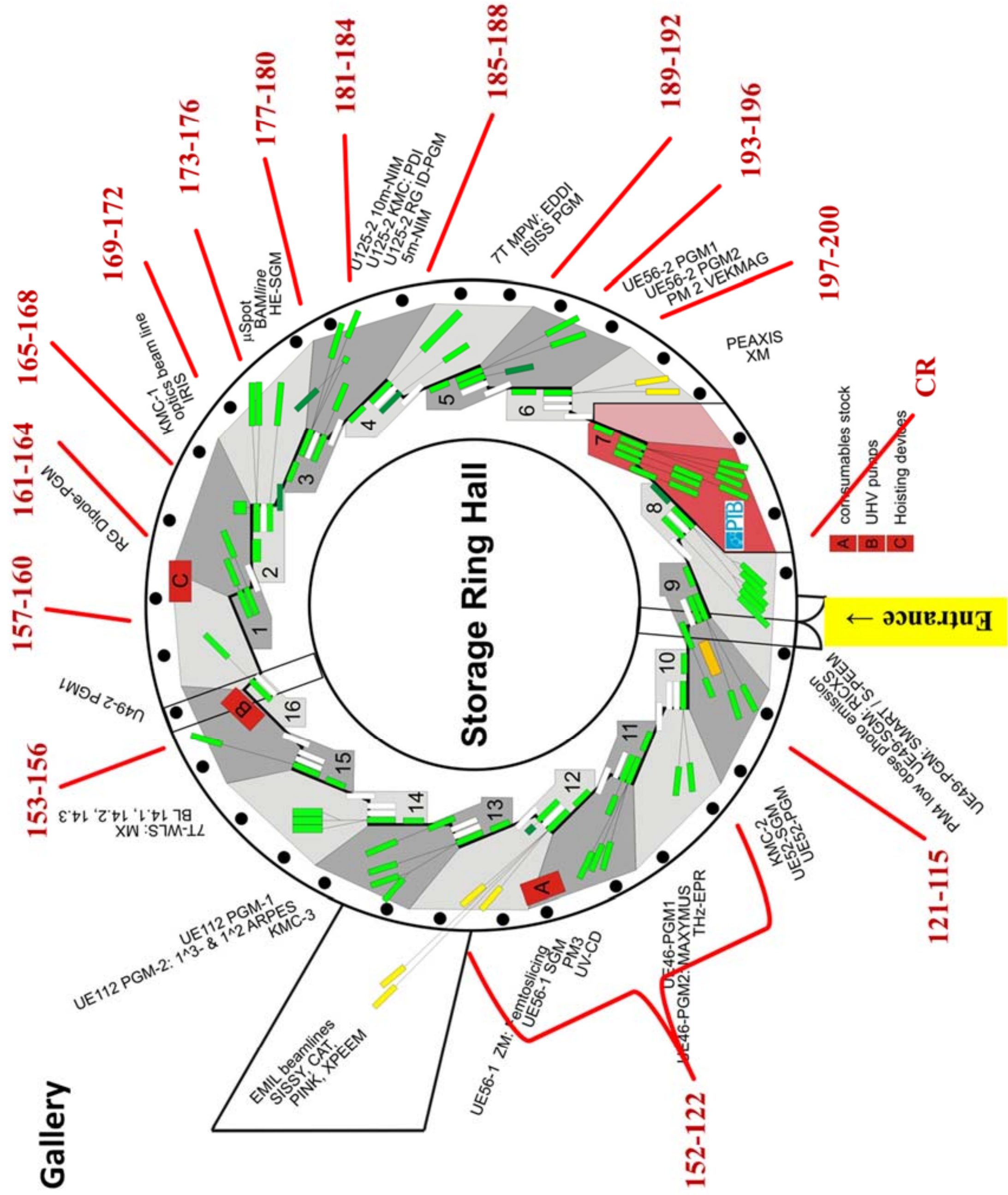

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Procedures for electing members of the HZB User Committee

The user representatives for the HZB User Committee are elected online by eligible users **via the HZB access portal GATE**:

https://www.helmholtz-berlin.de/user/gate/index_en.html

The voting period for the User Committee 2016 is
26. November 2016 [00:01] – **9. December 2016** [23:59]

Eligible users are defined as users of HZB's large-scale facilities, BER II and BESSY II, who have been actively registered on the HZB access portal GATE as a proposer, co-proposer or user during the three years immediately preceding the election.

All eligible users have been informed in advance by email by the User Committee election Committee. In order to be able to vote, the users must be registered in GATE.

List of candidates

Dahint, Reiner	Ruprecht-Karls-Universität Heidelberg, Deutschland	Physicist Methods: Neutron reflectometry, XPS Areas of interest: Biosensors and biomaterial interfaces **Neutrons**
Faelber, Katja	Max-Delbrück-Centrum für Molekulare Medizin, Deutschland	Physicist Methods: X-ray crystallography Area of interest: Structural biology **Photons**
Papp, Christian	Friedrich-Alexander-Universität Erlangen-Nürnberg, Deutschland	Chemist Methods: XPS, NEXAFS, ARPES Areas of interest: Chemistry on surfaces, 2d systems, energy storage concepts **Photons**
Schmidt, Harald	Technische Universität Clausthal, Deutschland	Physicist Methods: NR, GI-XRD, XRR, SAXS Area of interest: Material science with a focus on solid state kinetics **Neutrons**

Procedures for electing members of the HZB User Committee are organized and supervised by an independent election committee consisting of one member of the HZB User Committee, one representative of HZB User Coordination and one representative of the Scientific Director's Office at HZB. The election committee processes the proposals and nominates the final candidates for election.

The members of the current election committee are:

Antonia Schmitz-Antoniak	Forschungszentrum Jülich	Member of the User Commitee
Olaf Schwarzkopf	HZB	Representative of the Scientific Director's Office
Astrid Brandt	HZB	Representative of the HZB User Coordination

Friends of Helmholtz-Zentrum Berlin e.V.

The purpose of the Association of Friends of Helmholtz-Zentrum Berlin includes the support of the development of science and research, especially by the support of scientific activities at BESSY II. The association is a link between HZB and the general public and it shall develop the cooperation between HZB, its friends and sponsors and other national and international institutions. In particular, it is dedicated to support young scientists.

Main activities of the association include the annual bestowals of science awards. In memory of the former scientific director of BESSY, who died in September 1988, the association awards annually the Ernst-Eckhard-Koch-Prize. This prize is given for outstanding Ph.D. theses completed during the current or past year in the field of research with synchrotron radiation and performed at either BESSY II or HASYLAB (Hamburg) as the main places of activities of Ernst-Eckhard Koch. Furthermore, the association bestows the Innovation-Award on Synchrotron Radiation since 2001, which is announced Europe wide for an outstanding technical achievement or experimental method that promises to extend the frontiers of research with synchrotron radiation.

All natural or juristic persons may become member of the association. The regular annual membership fee amounts to 10 € for undergraduate and graduate students, 40 € for other natural persons and, as a rule, 150 € for juristic persons. In its work, the association depends also on donations which can also be addressed with a specific purpose, such as "Ernst-Eckhard-Koch-Prize" (Account-No.: 414 44 40 at the Deutsche Bank AG, BLZ 100 700 00). Fees and donations are enjoying tax privileges.

If somebody else feels associated with Helmholtz-Zentrum Berlin and its circle of friends we kindly ask him to support our activities by becoming a member.

The Board of the Association

An den Vorstand
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12489 Berlin
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e-mail: freundeskreis@helmholtz-berlin.de
Internet: http://www.helmholtz-berlin.de/freundeskreis

Mitgliedschaft

Hiermit beantrage ich die Aufnahme in den Verein Freundeskreis Helmholtz-Zentrum Berlin e.V.

Membership

Herewith I apply for admission to the Association Friends of Helmholtz-Centre Berlin

Angaben zur Person / personal data	
	Anrede: / salutation: Nachname: / last name: Vorname: / first name:
	Geburtsdatum: /date of birth: (DD-MM-YYYY) Herkunftsland:/Staatsangehörigkeit: /nationality
	Titel: / title: Berufsbezeichnung: / profession:
Institution / institution	
Name: / name:	
Abteilung: / department:	
Straße: / street:	
PLZ: / zip: Ort: / city: district:	
Land: / country:	
Telefon: / phone: Fax: / fax:	
Homepage: / e-mail: homepage of institution:	

Die jährlichen Mitgliedsbeiträge betragen zur Zeit für natürliche Personen EUR 40,-, für juristische Personen EUR 150,-, EUR 100,- oder EUR 50,-, für Studenten EUR 10,-. / The regular annual membership fees amount to EUR 40,- for natural persons, EUR 150,–/100,-/50,- for legal entities, EUR 10,- for students.

Art der Person: / Character of person: natural person ______ legal entity ______
Mitgliedsbeitrag : / Membership fees: Euro ____________

Im Rahmen freiwilliger Höherstufung/ voluntary upgrading: Euro ____________

Datum: / date: Unterschrift: / signature:

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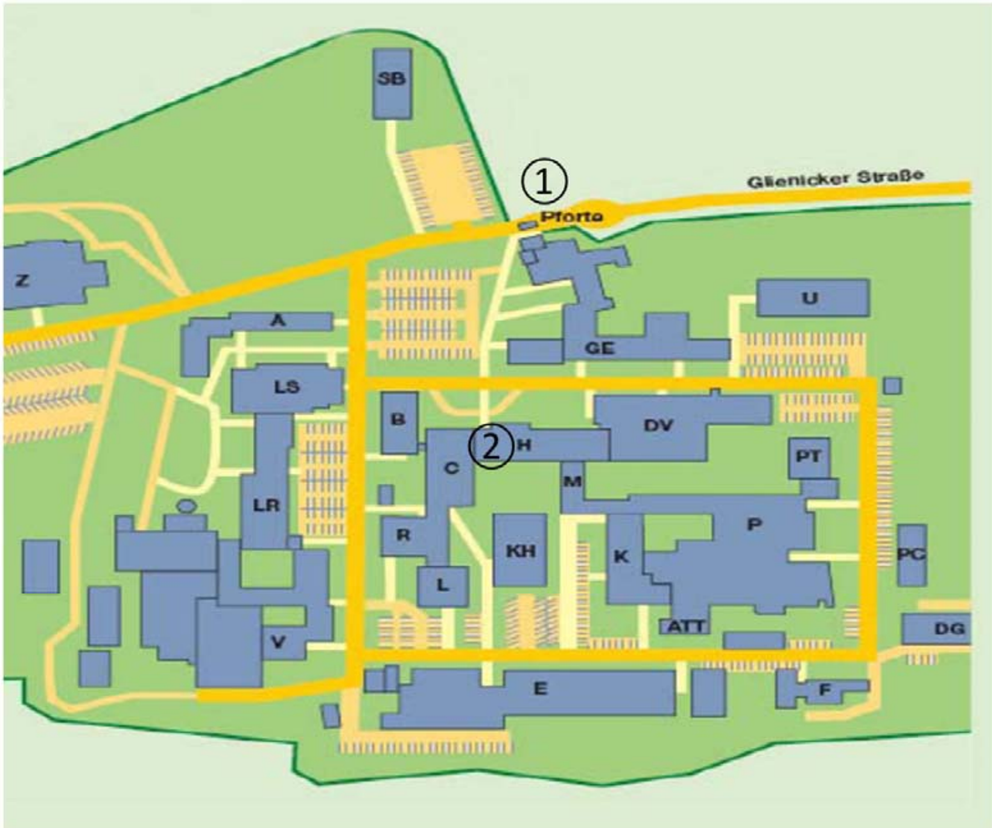
Helmholtz-Zentrum Berlin
Lise-Meitner Campus
Wannsee



① Main entrance
② Lecture building (H): LMC-Foyer
Cafe Jahn
Lecture Hall

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14109 Berlin

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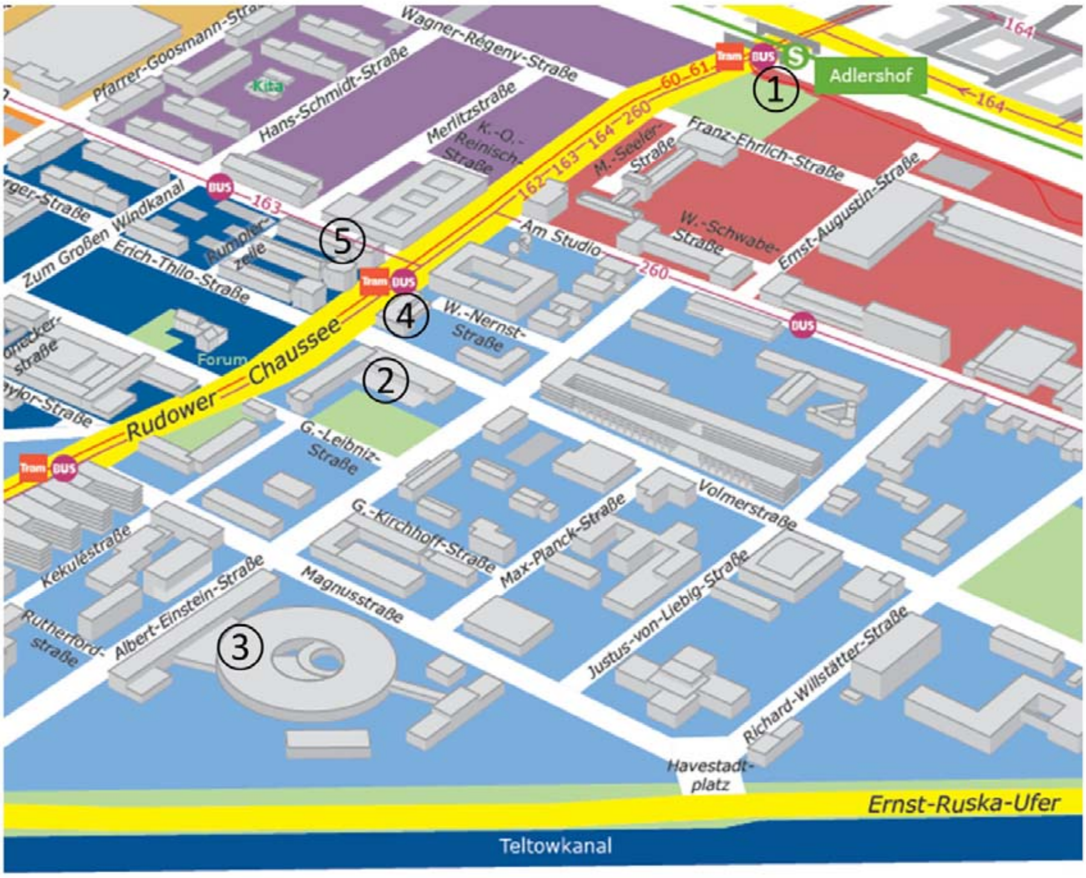
Helmholtz-Zentrum Berlin
Wilhelm Conrad Röntgen Campus
Adlershof



① Train Station Adlershof
② Wista centre: Registration
Bunsen Auditory
Vendor Exhibition
③ BESSY II Storage Ring Hall: Poster Session

Hotels:
④ Dorint
⑤ Airporthotel

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HZB Helmholtz Zentrum Berlin

Next deadline for submission:

1 March 2017

Call for Proposals 2017/II

HZB kindly invites you to submit proposals for the next allocation period from August 2017 to February 2018 for BESSY II and BER II.

Beamtime applications may only be submitted via the General Access Tool GATE:

http://hz-b.de/gate

For guidance in writing a proposal, please refer to the online Guide for beamtime application:

http://hz-b.de/beamguide

http://hz-b.de/proposals

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