HZB Helmholtz Zentrum Berlin

SEVENTH JOINT BER II AND BESSY II USER MEETING

Dec. 9-11, 2015

Key Note Lecture:
Petra de Jongh (Uni Utrecht)
Public Lecture:
David Cahen (Weizmann Inst.)

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

Invited talks:
Matthias Bernien (FU Berlin)
Matthew Harrington (MPIKG)
Mathias Kläui (Uni Mainz)
Tobias Lau (HZB)
Jörg Libuda (Uni Erlangen)
Claire Nichols (Uni Cambridge)
Hideaki Ogata (MPI Mühlheim)
Benjamin Stadtmüller (TU Kaiserslautern)
Simon Thiele (Uni Freiburg)
Kamil Wojciechowski (TU Warschau)

Satellite Foresight Workshops:

- **Tender X-rays in MX (Dec. 11)**
- **THz to soft X-ray (Dec. 7 to 8)**

December 9 to 11, 2015
Wilhelm-Conrad-Röntgen Campus, Berlin-Adlershof
WISTA
Lise-Meitner-Campus, Berlin-Wannsee

https://www.helmholtz-berlin.de/user/usermeetings/user-meeting-2015/index_en.html

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für Materialien und Energie GmbH

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Dear friends and users,

Welcome to the 7th *Joint BER II and BESSY II User Meeting of HZB*, which brings together users of our neutron and synchrotron sources at our sites in Berlin Wannsee and Adlershof.

The operation of the synchrotron source BESSY II has been characterized by a stable and brilliant photon flux in full top-up mode. In the process of continuously improving and up-grading beamlines as well as installing new instruments for our users, we are pleased to announce, that the LowDosePhotoemission Station and the new beamline XPP-KMC-3 are fully operational and the 7T-MPW with its station EDDI is back in full user service.

The construction of the building as well as the set-up of the analytics cluster of the Energy Materials in-situ Laboratory at BESSY II (EMIL@BESSYII) has been completed, and the first of its two undulators has been implemented in the storage ring; the related beamlines are about to be set-up. EMIL@BESSYII, which is operated in collaboration with the Max Planck Society, will offer new possibilities for in-situ energy materials research.

Important projects for the future of the BESSY II facility are making good progress; amongst them are the relocation of the U41 undulator and its associated beamlines U41-PGM and TXM, the up-grade of the MultiColourPES end-station by a coincidence ARTOF instrument (coESCA), the construction of the Russian-German Undulator beamline, and of the ENERGIZE beamline together with the Humboldt-Universität zu Berlin.

HZB has been continuing its series of foresight workshops which establish a discussion on future projects and research activities with current and future users from universities, research institutes, and industry. Aim of the dialogue is to discuss future scientific fields and the related expectations, needs and requirements for cutting edge science with synchrotron radiation. The first three workshops on “Tender X-Rays” with more than 80 participants, on “Pico-to-Femto – time resolved studies at BESSY II” with more than 170 participants and on “Imaging” with more than 130 participants showed that our users strongly engage in our development and contribute actively to these important discussions. Two foresight workshops, namely “THz-to-Soft X-Rays” and “Tender X-Rays in MX”, are taking place as satellites to this User Meeting. We are looking very much forward to continuing the series foresight workshops and the discussion with our users in further workshops on Accelerators and Energy Materials Research in 2016.

The neutron source BER II resumed operation in February 2015. With the start of user operation at the unique HFM/EXED instrument, HZB is making available the strongest continuous field for neutron scattering experiments worldwide.

This year's *Joint User Meeting* is highlighted by the keynote lecture by Petra de Jongh on "The stability of supported transition metal catalysts" and the public lecture by David Cahen on "Science: Bridge over troubled water". 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 young scientists presenting their research. For the first time, a science slam rounds up the young scientist's sessions this year.

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 9th, 2015 :
Young Scientists 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 – 15:30	**Synchrotron Session**	Bunsen Auditorium
14:00	*Thomas Frederking (HZB)* **Welcome**	
14:10	*Andreas Jankowiak (HZB)* **BESSY II: Accelerator and BESSY VSR**	
14:30	*Alexander Föhlisch (HZB)* **BESSY II: Photon Science and Instrumentation**	
14:50	*Simone Raoux (HZB)* **EMIL**	
15:10	*Florin Radu (HZB)* **VEKMAG**	
15:30	*Johannes Bahrdt (HZB)* **Short Period Undulator Development**	
15:50 – 16:05	**General Discussion**	Bunsen Auditorium
16:05 – 16:30	**Coffee Break**	WISTA Centre
16:30 – 18:00	**Young Scientist Session**	Bunsen Auditorium
16:30	*Ida Josefsson (Stockholm University)* **Ab initio Theorie für soft X-ray XAS und RIXS**	
16:45	*Maria Ekimova (MBI)* **A Flatjet System for Soft X-Ray Spectroscopy in the liquid phase**	
17:00	*Martin Bluschke (MPI FKF Stuttgart)* **Magnetic Interactions in Atomically Thin Nickelate/Scandate Heterostructures**	
17:15	*Manuela Gorgel (LMU München)* **Against the Odds? De-novo Structure Determination of a Single Cysteine Bridge Protein**	
17:30	*Francesca Ciccullo (University of Tübingen)* **Thin films of organic radicals: towards magnetism in purely organic materials**	
17:45	*Henriette Maaß (University of Würzburg)* **Resonant Photoelectron Spectroscopy of Strongly Spin-Orbit Coupled Systems**	
18:30-21:00	**HZB Science Slam**	Bunsen Auditorium

Thursday, December 10th, 2015 :
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** *Petra de Jongh (Universiteit Utrecht)* **The stability of supported transition metal catalysts**	
10:10 – 10:40	**Coffee Break and Vendor Exhibition**	WISTA Centre
10:40 – 12:20	**Oral Presentations I**	Bunsen Auditorium
10:40	*Matthias Bernien (FU Berlin)* **Highly Efficient Thermal and Light-Induced Spin-State Switching of an Fe(II) Complex in Direct Contact with a Solid Surface**	
11:00	*Claire Nichols (University of Cambridge UK)* **Nanopaleomagnetism of meteoritic Fe–Ni studied using X-ray photoemission electron microscopy**	
11:20	*Mathias Kläui (University of Mainz)* **X-ray based imaging of synchronous domain wall motion dynamics**	
11:40	*Tobias Lau (HZB)* **Maximum Spin Polarization in Chromium Dimer Cations as Demonstrated by X-ray Magnetic Circular Dichroism Spectroscopy**	
12:00	*Simon Thiele (Albert-Ludwigs-Universität Freiburg)* **Carbon binder domain at multiple scales and tomographic reconstructions**	
12:20 – 13:30	**Lunch Break**	(Canteens on site)
13:30 – 15:10	**Oral Presentations II**	Bunsen Auditorium
13:30	*Hideaki Ogata (MPI Mühlheim)* **Hydrogens detected by subatomic resolution protein crystallography in a [NiFe] hydrogenase**	

13:50	*Benjamin Stadtmüller (TU Kaiserslautern)* **Unexpected interplay of bonding height and energy level alignment at heteromolecular hybrid interfaces**	
14:10	*Kamil Wojciechowski (TU Warsaw)* **Effect of hydration of sugar groups on adsorption of Quillaja bark saponin at air/water and Si/water interfaces**	
14:30	*Matthew Harrington (MPIKG)* **Harnessing X-rays to elucidate structure-function relationships in a tough and self-healing biological fiber**	
14:50	*Jörg Libuda (University of Erlangen)* **Surface Science and Model Catalysis with Liquid Organic Hydrogen Carriers**	
15:10 – 15:40	**Coffee Break and Vendor Exhibition**	WISTA Centre
15:40 – 15:50	**Report from the User Committee**	Bunsen Auditorium
15:50 – 17:00	**Bestowal of Prizes: Friends of Helmholtz-Zentrum Berlin e.V.** *(Chair: M. Richter)*	Bunsen Auditorium
17:00 – 18:00	**Public Lecture** *David Cahen (Weizmann Institute)* **Science: A bridge over troubled waters**	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 11th, 2015:
Young Scientists and Neutron Day

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

8:30-9:00	**Registration**	**(LMC-Foyer and Café Jahn)**
9:00 – 10:30	Neutron Session	(Lecture Hall)
9:00	*Anke Kaysser-Pyzalla (HZB)* **Opening**	
9:10	*Oleksandr Prokhnenko (HZB)* **HFM/EXED - high magnetic field facility for neutron scattering**	
9:30	*Margarita Russina (HZB)* **TOF spectrometer NEAT at Helmholtz Zentrum Berlin – a powerful tool for energy materials research**	
9:50	*Michael Tovar (HZB)* **The FALCON-Laue-Diffractometer**	
10:10	*Matthias Ballauff (HZB)* **V16 – A versatile Time-of-flight small-angle neutron instrument**	
10:30 – 11:00	Coffee Break	(Café Jahn)
11:00 – 12:30	Young Scientists Session	(Lecture Hall)
11:00	*Ben Kent (HZB)* **Localization of disaccharides in partially hydrated DOPC bilayers: insights into cryoprotective mechanisms**	
11:15	*Eusebio Solorzano (University of Valadolid)* **Neutron and X-ray imaging in polymeric materials: a complementary understanding under different condition**	
11:30	*Nathalie Kunkel (Universität Leipzig)* **Hydrogenation properties of $Li_xSr_{1-x}AlSi$ studied by quantum-chemical methods** ($0 \leq x \leq 1$) and in-situ neutron powder diffraction ($x=1$)	
11:45	*Kimiya Hemmesi (Fraunhofer Institut Freiburg)* **Numerical Description of Welding Residual Stress in Tubular Joints and the Corresponding Experimental Investigations by Means of X-Ray, Synchrotron and Neutron Diffraction Methods**	
12:00	*Carsten Pohlmann (FHI IFAM)* **Neutron Imaging for Hydrogen Storage - Hydride-Graphite Composites during cyclic Hydrogenation**	
12:15	*Peter Nestler (Uni Greifswald)* **Diffusional Response of Polyelectrolyte Multilayers to Salt Annealing and Influence of Diffusion Barriers**	
12:30 – 14:00	**Poster Session and Lunch**	(Café Jahn)

Abstracts of the Young Scientist Session at the Synchrotron Day

Wednesday, 9th of December

Ab Initio Theory for Soft X-ray XAS and RIXS

Ida Josefsson[1]

1 Stockholm University, Sweden

With the development of light sources, the information available from x-ray spectroscopy increases, and advanced theoretical methods are needed to aid the interpretation of the fine details in the experimental spectra. We use high-level quantum chemistry to simulate x-ray spectra.

L-edge x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) map the electronic structure through electronic excitations from the 2p core to the unoccupied d levels and fluorescent decay of the core hole. X-ray spectroscopic techniques are well suited to study the electronic structure of transition metal complexes with element specificity. Such compounds are complex systems, and the simulated core-level spectra must be computed with a method that properly treats multiplet effects arising due to electron–electron correlations, as well as strong spin–orbit coupling of the core hole.

Changes in the local electronic structure of a transition metal complex during a chemical process can be studied on the femtosecond timescale with time-resolved XAS and RIXS, in combination with accurate theoretical modeling. Since the process may involve transient and highly distorted intermediate electronic states, it is desirable that the theoretical method includes the necessary effects ab initio. We show that an approach based on a multiconfigurational SCF wavefunction gives a good description of the L-edge spectra for transition metal complexes in solution, even with reactive states involved.

References:
[1] JPCL, 3, 3565, (2012),
[2] JPCB, 117, 16512, (2013),
[3] JPCL, 3, 1695 (2012),
[4] Nature, 520, 78, (2015)

M. Ekimova 9.12.15, 16:45

A Flatjet System for Soft X-Ray Spectroscopy in the liquid phase

M. Ekimova[1], W. Quevedo [2], M. Faubel[3], Ph. Wernet[2] and E. T. J. Nibbering[1]

1 Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany
2 Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz Zentrum Berlin for Materials and Energy GmbH, Germany
3 Max Planck Institute for Dynamics and Self-organization, Germany

We present[1] a liquid flatjet system as a new approach to perform soft X-ray spectroscopy in solution phase. The flatjet set-up is based on the phenomenon of formation of liquid sheets upon collision of two identical laminar jets.[2-4] Colliding single water jets, coming out of the nozzles with 50 μm orifices, under an impact angle of 48° leads to double sheet formation, of which the first sheet is 6 mm long and 1 mm wide. We determine the flatjet thickness under vacuum conditions ($<10^{-3}$ mbar), measuring the absorbance of liquid water at the oxygen K-edge and comparing them with the tabulated data from the Henke tables.[5] We characterized the thickness at atmospheric pressure using the interferometric method and IR transmission. We show that the thickness varies between 1.4 – 3 μm depending on the position at the sheet surface. A catcher unit facilitating the recycling of the solutions allows for measurements on smaller sample volumes (~ 10 ml), making it a clear technological advance compared to previously reported single liquid jet systems[6], where the liquid solution is guided towards cooling traps in the vacuum chamber. We demonstrate the potential of the flatjet set-up by presenting measurements on the nitrogen K-edge of aqueous NH_4^+ recorded directly in transmission mode. Our results suggest the high potential of using liquid flatjets in steady-state and time-resolved soft X-ray spectroscopy.

References:
[1] Struct. Dyn., 2, 054301, (2015),
[2] Proc. Roy. Soc. A, 259, 1, (1960),
[3] J. Fluid Mech., 511, 285, (2004),
[4] J. Fluid Mech., 549, 273, (2006),
[5] At. Data. Nucl. Data Tables, 54, 181, (1993),
[6] Chem. Rev., 106, 1176, (2006).

M. Bluschke 9.12.15, 17:00

Magnetic Interactions in Atomically Thin Nickelate/Scandate Heterostructures

M. Bluschke[1,2], A. Frano[1,2], E. Schierle[2], G. Christiani[1], E. Weschke[2], E. Benckiser[1], B. Keimer[1]

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2 Helmholtz-Zentrum Berlin für Materialien und Energie,
Wilhelm-Conrad-Röntgen-Campus BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Transition metal oxide heterostructures represent a rich platform for the study of correlated electron physics [1]. In particular, heterostructuring techniques allow for the manipulation of the collective phase behaviour of correlated electron systems via mechanisms such as epitaxial strain and quantum confinement [2,3]. Here resonant elastic x-ray scattering is used to probe the evolution of magnetic order in epitaxial superlattices of ultrathin $LaNiO_3$ and $DyScO_3$ layers grown on (110) oriented $DyScO_3$ substrates. At low temperatures a complex magnetic structure emerges, distinct from those of the constituent bulk materials. A *non-collinear* spin spiral antiferromagnetic order characterized in *Pbnm* notation by the wavevector **k** = (½ 0 ½) develops below 100 K among the Ni spins [2,3], and at lower temperatures a *collinear* antiferromagnetic order with the same wavevector is induced across the interface at the Dy sites. Below the Dy ordering temperature, it is demonstrated that a fully reversible switching of the Ni spin spiral polarization plane is achieved via the application of an external magnetic field. This phenomenon occurs as a result of the interface to $DyScO_3$, and has not previously been observed in other $LaNiO_3$ containing heterostructures. Magnetic switching mechanisms such as this are of great relevance for technological applications, and may pave the way towards studies in the largely unexplored field of antiferromagnetic metal spintronics.

References:
[1] Hwang, H. Y. *et al.,* Nature Mater. **11**, 103–113 (2012)
[2] A. V. Boris *et al.*, Science **332**, 937 (2011)
[3] A. Frano *et al.*, Phys. Rev. Lett. **111**, 106804 (2013)

Against the Odds? *De-novo* Structure Determination of a Single Cysteine Bridge Protein

Manuela Gorgel[1,2], Andreas Boeggild[1], Jakob Jensen Ulstrup[1], Manfred S. Weiss[3], Uwe Mueller[3], Poul Nissen[1] and Thomas Boesen[1]

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2 Gene Center, Ludwig-Maximilians-University Munich, Feodor-Lynen-Strasse 25, D-81377 Munich, Germany.
3 Helmholtz Zentrum Berlin für Materialien und Energie, Macromolecular Crystallography (HZB-MX), Albert-Einstein-Strasse 15, D-12489 Berlin, Germany.

Exploiting the anomalous signal of the intrinsic sulfur atoms to phase a protein structure is advantageous, as ideally only a single well-diffracting native crystal is required. However, sulfur is a weak anomalous scatterer at the typical wavelengths used for X-ray diffraction experiments and therefore, sulfur SAD data sets need to be recorded with a high multiplicity. In this study, we have determined the structure of a small pilin protein by S-SAD despite several obstacles such as a low anomalous signal (theoretical Bijvoet ratio of 0.9% at 1.8 Å), radiation damage induced reduction of the cysteines, and a multiplicity of only 5.5. The anomalous signal was improved by merging three data sets from different volumes of a single crystal yielding a multiplicity of 17.5 , and it added a sodium ion to the substructure of anomalous scatterers. In general, all data sets balance around threshold values for a successful phasing strategy. In addition, we present a collection of statistics on structures from the PDB that were solved by sulfur SAD and compare them with our data. Looking at the quality indicator R_{anom}/R_{pim}, we noted and hereby report an inconsistency on the documentation of the anomalous *R*-factor.

F. Ciccullo 9.12.15, 17:30

Thin films of organic radicals: towards magnetism in purely organic materials

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Stable organic radicals that can be defined as metal-free magnets carrying at least one unpaired electron, have recently gained great attention for a variety of applications including spintronics and memory elements. For a long time these molecules have been considered highly reactive and difficult to handle. But, since the first stable organic radical was discovered, many efforts have been focused on the synthesis of radicals with sufficient chemical stability under normal laboratory conditions. However, little attention has been paid to their thin film stability, although this property is an essential prerequisite in electronics.
Here, we report on thin films based on a new stable Blatter radical, which has been designed with the purpose of obtaining not only chemically stable radical, but also stable thin films. We investigated thin film properties and stability by means of a multi-technique approach, combining X-ray photoelectron spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS) carried out with the Angle Resolved Time Of Flight (ArTOF) electron analyser, to explore in situ the electronic structure of the thin films. The magnetic character of the thin films was proved ex situ by electron paramagnetic resonance (EPR) spectroscopy. Contrary to already existing radical derivatives, our results indicate that the radical has remarkable magnetic and stability properties, confirming the effectiveness of our methodology to introduce this class of materials into the real world of technology.

References:
[1] Chem.-Eur. J.,19,3445-3450,(2013),
[2] ACS Appl. Mater. Interfaces,5,13006-13011,(2013),
[3] ACS Appl. Mater. Interfaces,7,1685-1692,(2015)

Resonant Photoelectron Spectroscopy of Strongly Spin-Orbit Coupled Systems

Henriette Maaß[1], Hendrik Bentmann[1], Thiago R. F. Peixoto[1], Christoph Seibel[1] and Friedrich Reinert[1]

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Strong spin-orbit coupling leads to a lifting of the spin degeneracy of the electronic structure and the emergence of novel topological phases in non-centrosymmetric environments, such as interfaces or surfaces. Using resonant angle-resolved photoemission experiments we have investigated the spin-polarized electronic structure in topological insulator films and surface alloys with giant Rashba splitting.
In my presentation I will focus on the surface alloy $BiAg_2$/Ag(111), which exhibits one of the largest known spin-splittings in its surface electronic structure[1,2]. Our data reveals pronounced momentum dependent modulations of the photoemission intensity in the 6p derived surface states, when the photon energy is tuned across the Bi 5d core level excitation. Interestingly, the intensity variations are highly sensitive to the spin-polarization in the ground state band structure. In particular a complete suppression of spectral weight of spin-up and spin-down valence bands occurs for energies shortly below the Bi $5d_{5/2}$ and the $5d_{3/2}$ core level excitations, respectively. At the same time a considerable modification of the photoelectron spin-polarization can be observed.
We interpret these results in terms of a spin-selective effect in resonant photoemission from spin-polarized surface states that—in particular when combined with the element-specificity of the resonant photoemission process—may proof useful for a variety of other material systems.

References:
[1] Ast *et al.*, PRL 98, 186807 (2007)
[2] Bentmann *et al.*, PRL 108, 196801 (2012)

Abstracts of the invited talks at the Science Day

Thursday, 10th of December

The stability of supported transition metal catalysts

Petra E. de Jongh[1]

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

Catalysts typically consist of supported metal nanoparticles (<10 nm). Metal nanoparticles have an inherent tendency to grow into larger crystallites, especially at increased temperatures and in reactive gas atmospheres, leading to a decrease in the specific metal surface area and hence activity. Recent advances using for instance in *in situ* electron microscopy, STM under low gas pressures and computational approaches yield information on the mechanisms and fundamentals of particle growth in model systems. However, relatively little is still known about the mechanisms of particle growth under real reaction conditions in 3D supported systems.

We study the growth of supported nanoparticles using 3D ordered mesoporous supports as a key tool. They allow mimicking realistic catalyst systems and conditions (100-400 °C, 1-50 bar pressure, H_2, CO, CO_2, alkenes, H_2O, O_2 feeds), while their highly defined morphology facilitates high precision in the variation of individual structural parameters. In this presentation I will highlight a few examples based on Cu, Ni and Co catalysts for synthesis gas conversion and methanation.[1-5] We vary particle parameters such as size, size distribution, and average particle density, but also collective properties such as the nanospatial distribution of the metal nanoparticles over the support, and support pore size, window size, connectivity (for instance 1D or 3D porosity), and surface. Our aim is to understand in detail the interplay of different structural parameters, and obtain information on the nature of the mechanism of particle growth (for instance Ostwald ripening versus particle migration and sintering versus removal of the active component) under given, realistic, catalysis conditions.

References:
[1] Nature Mater. 12, 23 (2013);
[2] ACS Nano 8, 2522 (2014);
[3] J. Am. Chem. Soc. 137, 7333 (2014);
[4] Angew. Chem. Int. Edit 126, 9647 (2014);
[5] Angew. Chem. Int. Edit. 54, 11804 (2015).

Science: A bridge over troubled waters

David Cahen[1]

1 Weizmann Institute of Science, Rehovoth, ISRAEL

I will present some examples, including contemporary ones, where science, specifically natural science, allowed / allows its practitioners to overcome strong differences in world-views, be they current political or territorial ones, or historical events to communicate (i.e., talk AND listen).

As long as the generally accepted language of science (observation-based, rather than purely Aristotelian) is not challenged (cf. genetics-evolution, physics, climate science), scientific discussions can provide a bridge where other means may fail.

Abstracts of the Oral Presentations at the Science Day

Thursday, 10th of December

Highly Efficient Thermal and Light-Induced Spin-State Switching of an Fe(II) Complex in Direct Contact with a Solid Surface

M. Bernien[1], H. Naggert[2], L. M. Arruda[1], L. Kipgen[1], F. Nickel[1], J. Miguel[1], C. F. Hermanns[1], A. Krüger[1], D. Krüger[1], E. Schierle[3], E. Weschke[3], F. Tuczek[2], and W. Kuch[1]

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2 Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Straße 2, 24098 Kiel, Germany
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany

Spin crossover (SCO) complexes possess a bistable spin state that reacts sensitively to changes in temperature or excitation with light. These effects have been well investigated in solids and solutions, while technological applications require the immobilization and contacting of the molecules at surfaces, which often results in the suppression of the SCO. I will present x-ray absorption measurements that evidence thermal and light-induced SCO of $[Fe(bpz)_2phen]$ molecules in direct contact with a highly oriented pyrolytic graphite surface. We are able to switch on the magnetic moment of the molecules by illumination with green light at T = 6 K, and off by increasing the temperature to 65 K. The light-induced switching process is highly efficient leading to a complete spin conversion from the low-spin to the high-spin state within a submonolayer of molecules. $[Fe(bpz)_2phen]$ complexes immobilized on weakly interacting graphite substrates are thus promising candidates to realize the vision of an optically controlled molecular logic unit for spintronic devices.

References:
[1] ACS Nano, 9, 8960 (2015)

C. Nichols 10.12.15, 11:00

Nanopaleomagnetism of meteoritic Fe–Ni studied using X-ray photoemission electron microscopy

Claire Nichols[1], James Bryson[2], Julia Herrero-Albillos[3], Florian Kronast[4], Richard Harrison[1]

1 University of Cambridge, UK
2 MIT, USA
3 Universidad de Zaragoza, Spain
4 HZB, Germany

Microstructural and geochemical studies of meteoritic metal have been instrumental in shaping our current views of differentiated planetesimals, providing constraints on their cooling rate, their size, the timing of their differentiation and their fractional crystallization and impact histories. The characteristic Widmanstätten microstructure, familiar to anyone who has looked at a polished and etched section of an iron meteorite with the naked eye, hides a nanoscale complexity that is revealed only with high-resolution electron microscopy – a legacy of stranded diffusion profiles, metastability, martensitic transformations, chemical segregation and ordering during slow cooling over millions of years on the parent body. The presence of magnetically soft bcc iron has traditionally lead to the meteoritic metal being dismissed as a reliable carrier of paleomagnetic information. However, we have shown that, under favourable circumstances, paleomagnetic information can be recorded and retained on a local scale within a unique nanoscale intergrowth called the cloudy zone. High-resolution XPEEM enables the magnetic states of the cloudy zone to be imaged and analysed quantitatively, opening up new avenues of research into the nanopaleomagnetism of a range of meteorites. Such studies are not only revealing new insight into the thermochemical properties of planetesimals in the early solar system, but provide us with unique opportunities to learn about how magnetic fields are generated on planetary bodies in general, and the underlying physics of the dynamo generation process itself.

References:
[1] EPSL, 388, (2014)
[2] EPSL, 396, (2014)
[3] Nature, 517, 7535, (2015)

X-ray based imaging of synchronous domain wall motion dynamics

Mathias Kläui[1,2]

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A wide range of future spintronic memory and logic devices require the ability to carefully control the motion of magnetic domain walls (DWs) [1]. Conventional DW manipulation approaches via in-plane magnetic fields lead to fast domain wall motion [2]. We have shown that we can displace domain walls in curved geometries reliably and we use geometrical variations to control the wall propagation and speeds and ascertain the potential landscape. However in-plane fields are not suitable for synchronous propagation of multiple DWs in a single wire as required for the racetrack, since adjacent walls have different spin-orientations and hence move in opposing directions, which leads to a loss of data when the DWs annihilate. An alternative is the use of current driven DW motion, which does facilitate synchronous DW motion, yet requires prohibitively large current densities. Here we demonstrate a radically different DW propagation scheme using out-of-plane field pulses which combines the efficiency of field-induced motion with the ability to move multiple walls synchronously [3]. This is achieved for in-plane magnetized transverse DWs of the same chirality through the application of asymmetric field pulses to a wire which incorporates regularly spaced pinning sites. An analytical model is developed to describe the system which reveals that the force on the DW is independent of the wall orientation but crucially depends on the time derivative of the applied magnetic field [3]. It is therefore possible to tailor the force on the DW by choosing the pulse rise and fall times and by applying asymmetric field pulses achieve net DW motion. This scheme is then successfully demonstrated in a realistic system via micromagnetic modelling. Finally, the concept is experimentally confirmed using scanning tunnelling x-ray microscopy [3].

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T. Lau 10.12.15, 11:40

Maximum Spin Polarization in Chromium Dimer Cations as Demonstrated by X-ray Magnetic Circular Dichroism Spectroscopy

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X-ray magnetic circular dichroism spectroscopy has been used to characterize the electronic structure and magnetic moment of Cr_2^+. Our results indicate that the removal of a single electron from the $4s\sigma_g$ bonding orbital of Cr_2 drastically changes the preferred coupling of the 3d electronic spins. While the neutral molecule has a zero-spin ground state with a very short bond length, the molecular cation exhibits a ferromagnetically coupled ground state with the highest possible spin of S=11/2, and almost twice the bond length of the neutral molecule. This spin configuration can be interpreted as a result of indirect exchange coupling between the 3d electrons of the two atoms that is mediated by the single $4s\sigma$ electron through a strong intraatomic 3d-4s exchange interaction. Our finding allows an estimate of the relative energies of two states that are often discussed as ground-state candidates, the ferromagnetically coupled $^{12}\Sigma$ and the low-spin $^2\Sigma$ state.

S. Thiele 10.12.15, 12:00

Carbon binder domain at multiple scales and tomographic reconstructions

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Lithium ion batteries are considered a central part of the solution to the energy transition challenge society is currently facing. Understanding battery microstructure and its relation to transport of reactants is pivotal to develop the next generation of battery systems.
Lithium ion battery electrodes consist of three phases: active materials (e.g. lithium cobalt oxide or lithium manganese oxide) for lithium storage, a carbon binder domain for electron conduction and a porous electrolyte phase for ion transport.
Tomographic analysis, in particular by synchrotron X-ray imaging, has proven to be a central technique to understand processes in active material particles of battery electrodes [1]. Those works however failed to reconstruct all three phases of battery electrodes as the carbon binder domain could not be imaged.
We present our studies that investigate the influence of the carbon binder domain on transport processes in lithium ion batteries. In the first part we present an approach to model different carbon binder domain morphologies within an active material reconstruction by X-ray tomography [2]. We show that all transport parameters strongly depend on carbon binder domain morphology. In the second part we present an approach to investigate multi-scale phenomena in transport processes by multiple imaging methods and a spatial statistical modeling approach [3]. We emphasize the importance to incorporate multi-scale phenomena in tomographic reconstructions of hierarchical materials.

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[3] Adv. Energy Mater.,4, 8, (2014)

Hydrogens detected by subatomic resolution protein crystallography in a [NiFe] hydrogenase

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Hydrogenases are metalloenzymes that catalyze the conversion of dihydrogen into protons and electrons and the reverse reaction, the generation of dihydrogen.[1] The oxygen-sensitive (standard) [NiFe] hydrogenase from sulfate reducing bacterium (*Desulfovibrio vulgaris* Miyazaki F) has been extensively characterized. Standard [NiFe] hydrogenaes are mainly composed of two subunits. The active site of [NiFe] hydrogenase is composed of the dinuclear Ni-Fe center, where the Fe ion is coordinated by non-protein ligands (1CO; $2CN^-$). Two thiolates of cysteine residues are bridging both metals. Furthermore, the Ni is coordinated to the two thiolates of cysteine residues in a terminal fashion. A third bridging ligand is found between the Ni and Fe atom, depending on the redox state. In the inactive form, a third bridging ligand (OH^-) is found between Ni and Fe.

Once the enzyme is activated, the bridging position is supposed to be vacant or bridged by a hydride.[2] Electron paramagnetic resonance (EPR) spectroscopy showed that a hydride is located in the bridge between Ni and Fe, which is lost upon illumination at cryogenic temperature.[3] A high-resolution crystallographic analysis of the fully reduced (Ni-R) state of [NiFe] hydrogenase F at 0.89 Å resolution will be presented. The subatomic resolution analysis revealed the presence of the hydride bridge at the [NiFe] active site.[4] Furthermore the CO and CN^- ligands could be identified and a protonated thiolate sulfur ligand of the Ni is postulated based on the electron density.

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Unexpected interplay of bonding height and energy level alignment at heteromolecular hybrid interfaces

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One crucial issue for the success of organic materials in electronic devices is our ability to design the interfaces between different active layers according to their functional purpose. While so far most studies focused on tailoring metal-organic interfaces by either exchanging the substrate material or by functionalizing organic adsorbates, we recently started to investigate mixed layers containing two different types of molecules.
For heteromolecular monolayer films of CuPc and PTCDA, we show that three long range ordered structures with different CuPc/PTCDA stoichiometry exist on the Ag(111) surface. Changing the molecular coverage of CuPc and PTCDA on Ag(111) results in different lattice parameters and hence allows us to tailor the lateral order of metal-organic hybrid interfaces [1]. Most remarkable, our angle resolved photoelectron spectroscopy recorded at BESSY II provide evidence for a significant change in the molecular valence structure which leads to a substrate mediated charge transfer from CuPc to PTCDA [2]. In addition, when comparing homo- and heteromolecular layers of these molecules, we find a systematic adsorption height adjustment between CuPc and PTCDA [2]. Similar trends were also observed for different combinations of prototypical molecules [3]. These experimental observations, i.e., the substrate mediated charge transfer and the adsorption height alignment, can be understood by density functional theory calculations and are the result of a mutual amplification of the charge-donating and –accepting character of both molecules in the heteromolecular film. We propose that these effects are of general validity for pi-conjugated molecules on noble metal surfaces.

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Effect of hydration of sugar groups on adsorption of Quillaja bark saponin at air/water and Si/water interfaces

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Adsorption of a natural glycoside surfactant Quillaja bark saponin (QBS) at the air/water and Si/water interfaces will be described using a combination of Neutron Reflectometry, Surface Pressure, Surface Dilatational Rheology, Infra-Red Attenuated Total Reflection Spectroscopy and Quartz Crystal Microbalance techniques. The adsorbed biosurfactant layers are predominantly elastic at the air/water interface and the NR results point to a strong hydration of the adsorbed layers (about 65% hydration, corresponding to about sixty molecules of water per one QBS molecule). The latter is most likely caused by the presence of multiple sugar groups constituting the glycone part of the QBS molecules. With a layer thickness of 19 Å, the adsorbed amount obtained from NR seems largely underestimated in comparison to the value obtained from the surface tension isotherm.
The adsorption isotherm of QBS on Si obtained from the QCM study reflects much lower affinity of highly hydrated and negatively charged saponin molecules to the Si/water interface. We postulate that at the air/water interface, QBS adsorbs through the triterpene aglycone moiety, in contrast to the more polar Si/water interface, where only weak hydrogen bonding between the glycone part and the surface silanol groups of Si drives QBS adsorption.
In the second part, interactions between a model phospholipid 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and QBS will be discussed from the point of view mixed Langmuir-Gibbs monolayers probed with neutron reflectivity and surface pressure techniques.

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M. Harringon 10.12.15, 14:30

Harnessing X-rays to elucidate structure-function relationships in a tough and self-healing biological fiber

Antje Reinecke[1], Clemens N.Z. Schmitt[1], Yael Politi[1], Luca Bertinetti[1], Peter Fratzl[1], Matthew J. Harrington[1]

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Biopolymeric materials such as spider silk and mussel byssus are important archetypes for the design of next-generation polymers because of their remarkable material properties and their environmentally friendly processing. Mussel byssal threads are biological fibers synthesized by mussels as an anchoring holdfast in wave-battered seashore habitats. Because the byssus is almost entirely composed of proteins, the material properties must arise from specific structural and biochemical properties of the protein building blocks comprising the material. In order to elucidate the underlying design principles of the mussel byssal thread mechanical properties, we have utilized a combined approach with wide-angle X-ray diffraction (WAXD), small-angle X-ray scattering (SAXS) and X-ray absorption spectroscopy (XAS) coupled to mechanical testing. Results of these studies provide a new comprehensive understanding of the roles of specific protein conformations, higher order hierarchical assemblies and unique cross-linking strategies in achieving the characteristic tough and self-healing behavior. Specifically, we highlight the importance of amyloid-like beta-sheet-rich protein domains that are stabilized by protein-metal coordination cross-links. These findings have a strong potential to inspire the future design of high performance polymers.

Surface Science and Model Catalysis with Liquid Organic Hydrogen Carriers

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2 Interdisciplinary Center Interface Controlled Processes and Erlangen Catalysis Resource Center, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Efficient energy storage technologies are essential for the future transition to renewable energy sources. Hydrogen is among the most promising energy vectors, but it requires high pressures or low temperatures to obtain sufficient energy densities. The associated technical issues can be overcome by chemical storage, for example in form of liquid organic hydrogen carriers (LOHCs). The LOHC concept is based on reversible catalytic hydrogenation of organic compounds. LOHC technology enables decentralized energy storage, i.e. it decouples energy production and consumption and, thereby, may help immensely to integrate renewable energies into our future energy mix.
In this contribution we provide an overview over recent surface science and model catalytic studies on different LOHC systems. Among the most prominent LOHC couples is N-ethylcarabzole/perhydro-N-ethylcarbazole, but there are many promising N-free alternatives such as benzoltoluenes and dibenzoltouenes. We have studied the dehydrogenation mechanisms and microkinetics of several LOHCs by synchrotron radiation high resolution X-ray photoelectron spectroscopy, infrared reflection absorption spectroscopy, temperature programmed desorption and molecular beam methods. Different model compounds were investigated both on Pt(111) and Pd(111) and on well-defined Pt and Pd supported model catalysts. In spite of the complexity of the molecular systems a large number of reaction intermediates could be identified. Also we have characterized the competing reaction pathways that can lead to degradation of the LOHC and to poisoning of the catalyst. Many of the observed reactions show characteristic dependencies on the particle size, the particle structure and on the catalyst material.

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Abstracts of the Young Scientist Session at the Neutron Day

Friday, 11th of December

Localization of disaccharides in partially hydrated DOPC bilayers: insights into cryoprotective mechanisms

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The prevailing view of membrane protection by sugars describes a close interaction between disaccharide and the lipid headgroups of bilayer membranes. This theory proposes the cryoprotective mechanism is based on sugars replacing water in the volume surrounding the lipid headgroups, thereby preventing a reduction in the area per lipid due to the strong compressive force that acts on the membranes during dehydration. This hypothesis is supported by indirect experimental methods[1] as well as molecular dynamics simulations[2] which point to accumulations of disaccharides, particularly trehalose, at the surface of lipid bilayers as evidence for this mechanism.

In this talk, we present results from neutron membrane diffraction measurements conducted on the V1 Membrane Diffractometer at HZB that show trehalose and sucrose distributions locate in the centre of the water layer. Furthermore, there is an absence of correlation between the headgroup position and the sugar distributions. These direct experimental results are clearly inconsistent with the above widely held cryoprotection theory, and support the view that osmotic and volumetric effects, combined with vitrification at high concentrations, maintain membrane separation and delay or avoid the onset of hydration forces known to alter lipid membrane phase behaviour[5]. The implications of these results for our understanding of natural anhydrobiosis and cryoprotection will be discussed.

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E. Solórzano 11.12.15, 11:15

Neutron and X-ray imaging in polymeric materials: a complementary understanding under different conditions

E. Solórzano[1], S. Pérez-Tamarit[2], J. Martin-de León[3], N. Kardijlov, I. Manke, A. Hilger, F. Wieder, M.A. Rodríguez-Pérez

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In this talk we will discuss on the possibilities of high resolution neutron tomography, in comparison to X-ray microCT. The neutron experiments have been carried out at the V7/CONRAD-2 imaging instrument located at the BER-II research reactor at HZB and compared to the images obtained in both in laboratory and synchrotron (BAMline, Bessy-II) X-ray microCT facilities. The recent developments of high-resolution neutron imaging at CONRAD beamline and the enhanced neutron attenuation of polymers relative to the X-rays encouraged these investigations. A better signal-to-noise ratio was found for the X-ray experiments in comparison with current neutron tomography. Nevertheless the contrast of polymeric materials in neutron imaging offered the possibilities of performing in-situ experiments inside high-pressure vessels (up to 200bar), thus monitoring in time the changes in the sample during a gas dissolution process.

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Hydrogenation properties of $Li_xSr_{1-x}AlSi$ studied by quantum-chemical methods ($0 \leq x \leq 1$) and in-situ neutron powder diffraction ($x = 1$)

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In-situ neutron powder diffraction studies of the Half-Heusler phase LiAlSi under high deuterium pressure were carried out at the D20, ILL and the E6, BerII. Furthermore, the solid solution series $Li_xSr_{1-x}AlSi$ and their hydrides $Li_xSr_{1-x}AlSiH$ were investigated by first principle calculations [1]. The lithium-free compound SrAlSi and SrAlSiH are well-known [2,3] and belong to the class of Zintl phases and polyanionic hydrides, respectively.
For the in-situ studies a single crystal sapphire high pressure cell developed by Kohlmann et al [4] was used in order to avoid a high background as it is usually observed for conventional high pressure cells. Up to deuterium pressures of 15 MPa and 550°C no evidence for the formation of a hydride $LiAlSiD_x$ was found. Instead a slow decomposition into LiD, Al and Si was observed. Theoretical calculations on hypothetical solid solution series $LixSr_{1-x}AlSi$ and $Li_xSr_{1-x}AlSiH$ suggest that for $0.7 > x$ the LiAlSi type structure is energetically stable, the SrAlSi type structure for lower values of x and, surprisingly, the hydrides $Li_xSr_{1-x}AlSiH$ favor the SrAlSiH type for all x. Positive energies of formation for LiAlSiH were obtained, both in the hypothetical cubic LiAlSiH structure type and the trigonal SrAlSiH structure type.

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Numerical Description of Welding Residual Stress in Tubular Joints and the Corresponding Experimental Investigations by Means of X-Ray, Synchrotron and Neutron Diffraction Methods

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In order to achieve fatigue resistant welded structures, it is necessary to manage and control welding process related factors which affect the fatigue strength. These factors are sometimes present as welding defects and sometimes as inevitable residual stresses which are unwanted by-products of welding processes. Having advanced predictive tools for accurate determining welding residual stresses will not only lead to the possibility of considering precise welding residual stress effects during life estimation, but also can be useful to have effective measures for the subsequent mitigation or modification processes on the welding residual stress fields.
The goal is to describe experimentally and numerically the welding residual stress field in welded tubular joints made of structural steel S355J2H. Residual stresses in cylindrical specimens with bead on tube welds were determined experimentally by means of x-ray, synchrotron and neutron diffraction techniques. SYSWELD software is used to calculate the welding residual stresses numerically. Obtained results from this early stage which include both thermal and metallurgical history, are used as input data for mechanical calculations afterward. The accuracy of the both thermal and structural models is validated through experiments for temperature distribution and residual stresses. Owing the complexity of this problem, well qualified measured data by using x-ray and neutron diffraction methods are required for the validation of numerical results. On the other hand, for a complete residual stress field determination a combination of the x-ray, synchrotron and neutron diffraction techniques are required. Particularly, the in-depth measurements by means of neutron diffraction are essential to reveal the total residual stress filed in the weldments.

Neutron Imaging for Hydrogen Storage - Hydride-Graphite Composites during cyclic Hydrogenation

Pohlmann Carsten[1,*], Herbrig Kai[2], Gondek Łukasz[3], Kardjilov Nikolay[4], Hilger André[4], Figiel Henryk[3], Manke Ingo[4], Kieback Bernd[5,6], Röntzsch Lars[5]

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Currently metal hydrides attract great interest among researchers due to their high volumetric storage capacity at moderate pressures of some ten bars. In this regard hydride graphite composites (HGC) offer a solution to overcome restricted heat and gas transfer properties of commonly used loose powder beds. Yet, to realize safe, efficient and compact hydrogen storage systems it is inevitable to generate a deep understanding of the materials behavior in order to draw conclusions for material as well as tank design.

This contribution deals with the in operando characterization of metal hydride composites (HGC) to ensure suitable hydrogen storage solutions based on this material set up. Neutron imaging (radiography and tomography) was used to thoroughly examine the composite materials during hydrogenation and dehydrogenation.

New information on the activation, swelling and hydrogenation behavior of HGC were deduced with the one of its kind neutron radiography and tomography setup at Helmholtz Center Berlin for Materials and Energy (HZB, BER II, CONRAD-Beamline V7). For example, within the first hydrogenation cycles a region of higher hydrogenation activity occurs which grows in size during cycling until the whole HGC participates. This allows valuable insights in the activation behavior of HGCs. Furthermore, this activation is accompanied by an irreversible volume expansion. In the following cycles a reversible volume change between the hydrogenated and dehydrogenated state was found. These findings allow drawing conclusions on technically relevant design criteria.

P. Nestler 11.12.15, 12:15

Diffusional Response of Polyelectrolyte Multilayer Films to Salt Annealing and Influence of Diffusion Barriers

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Polyelectrolyte multilayer films (PEMs) are made by adsorbing stratified layers of polyanions and polycations, linear poly(styrenesulfonate) (PSS), linear poly(diallyldimethylammonium) (PDADMA) and branched poly(ethylene imine) (PEI). Using selective PSS deuteration each film consists of a protonated and a deuterated compartment. During annealing in 1 mol/L NaCl the internal interface between these two compartments broadens due to interdiffusion. Via neutron reflectivity the distribution of protonated and deuterated PSS within the PEM is investigated, and the PSS diffusion coefficient is measured. Eventually the annealing leads to a uniform distribution of protonated and deuterated PSS throughout the film. Yet, if one polycation layer in the film centre is branched PEI, then this PEI layer serves as a diffusion barrier, which is impenetrable for up to 32 % of PSS macromolecules. The permeation rate of the remaining mobile PSS fraction is quantified. Additionally the equilibration time of the remaining mobile PSS fraction increases which is attributed to the low permeation rate through the barrier layer. Possibly, some PSS molecules have a conformation that hinders them to cross the barrier layer, or the barrier layer gets clogged.

Abstracts of Poster Session – Science Day at BESSY II

Thursday, 10th of December

0a Design and Synthesis of a Blatter Radical for Stable Thin Films

Ciccullo F, Gallagher N M, Ovsyannikov R, Rajca A, Casu M B

We have synthesized and characterized a derivative of the Blatter radical, bearing in mind the thermodynamic factors that govern thin film stability. We have proved our concept by investigating the electronic structure, the paramagnetic character, and stability of the films by in-situ photoelectron spectroscopy, ex-situ atomic force microscopy, and electron paramagnetic resonance spectroscopy.

0b Influence of Graphene on Charge Transfer between CoPc and Metals: The Role of Graphene-Substrate Coupling

Uihlein J, Polek M, Glaser M, Adler H, Balle D, Ivanovic M, Ovsyannikov R, Preobrajenski AB, Generalov AV, Chassé T, Peisert H

The electronic structure of cobalt phthalocyanine (CoPc) on Pt(111), graphene/Pt(111) and Au-intercalated graphene/Ni(111) is investigated by photoemission and X-ray absorption spectroscopy. The disturbance of the graphene electronic structure by interaction with underlying substrate accompanied by a doping of graphene has been found to affect electronic properties of adsorbed CoPc considerably.

0c Charge Transfer Dynamics from Ru Polypyridyl Complexes to ZnO and TiO2 Nanocrystalline Thin Films Studied by Means of Ultrafast XUV Photoelectron Spectroscopy

Borgwardt M, Wilke M, Kampen T, Mähl S, Spiccia L, Lange K,Kiyan I, Aziz E

ZnO represents a promising alternative compared to TiO_2 in DSSCs due to is much higher bulk electron mobility and the larger diversity in growth of nanostructured electrodes. However, energy conversion efficiencies are far from the record values of its TiO_2 counterparts. The aim of the present work is to employ the capabilities of ultrafast photoelectron spectroscopy to reveal possible reasons.

0d Depth-resolved photoemission study of Be2W and its interaction with O-Ions

Köppen M, Schmid K, Riesch J, Vollmer A, Linsmeier Ch

Fusion research aims at the exploitation of the deuterium-tritium reaction for energy production. Plasma processes induce surface reactions at the first wall of a fusion reactor. These processes can be investigated depth-resolved via our forward-calculation model for energy-resolved photoelectron spectroscopy. With this method the interaction of O-ions with Be_2W is analysed.

3 The Optical and Thermal Spin State Switching of Fe(bpz)2bipy on Surfaces

Kipgen L, Naggert H, Bernien M, Nickel F, Arruda L, Britton A, Kopprasch J, Xu Q, Tuczek F, Kuch W

The control of spin state of molecules from the high spin state HS to the low spin state LS or vice versa by thermal and optical means is envisioned to provide the building blocks for future spintronic devices.To this end, the understanding of the nature and behavior of the interaction of molecules and surfaces is crucial.

4 Surface-orientation-dependent spin quenching of adsorbed Co porphyrin molecules

Arruda L M, Bernien M, Nickel F, Kipgen L, Hermanns C F, Miguel J, Krüger A, Krüger D, Hatter N, Kopprasch J, Xu Q, Kuch W

We have investigated submonolayers of Co octaethyl porphyrin molecules on Cu(001), Cu(111) and Au(111) surfaces by means of x-ray absorption spectroscopy and x-ray magnetic circular dichroism in an external magnetic field of 6 T at a temperature of 5 K. We find the Co magnetic moment quenched when the molecule is adsorbed on Cu(111) and Au(111), but not on Cu(001).

4a XAS, XMCD, and Multiplet Calculations of Paramagnetic Dy Complexes on Au(111)

Bernien M, Stoll P, Rolf D, Nickel F, Xu Q, Hartmann C, Umbach T R, Kopprasch J, Ladenthin J N, Schierle E, Weschke E, Czekelius C, Franke K J, Kuch W

By means of XAS and XMCD at T = 4.5 K and B = 6 T we find that Dy-tris(1,1,1-trifluoro-4-(2-thienyl)-2,4-butanedionate) molecules on Au(111) display a magnetic easy-axis parallel to the surface. Upon adsorption, the coordination of the Dy ion by its three two-dentate ligands is deformed due to the interaction with the surface, stabilizing an unusual M_J = 15/2 ground state.

5 MAXYMUS at low temperatures

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

Using a scanning x-ray microscope the magnetic flux line density within a superconductor can be imaged with high spatial resolution. The stray field of the superconductor is responsible for a locally varying XMCD-signal in an adjacent soft ferromagnetic sensor layer. Spatially resolved XMCD images are obtained by the total electron yield (TEY) mode of the low temperature setup in the SXM MAXYMUS.

6 Ptychographic imaging at MAXYMUS X-ray Microscope

Bykova Iu, Weigand M, Bechtel M, Gräfe J, Goering E, Schütz G

MAXYMUS is an UHV STXM operated by the MPI IS at the Bessy II. Recently it was upgraded with a new fast in-vacuum CCD camera. High readout speed up to 450 Hz and RMS noise per pixel less than 3e- allow efficient ptychographic imaging that provides drastic increase in resolution. We will present the first results of commissioning of the CCD camera and ptychographic imaging at MAXYMUS.

7 Observation of Room Temperature Magnetic Skyrmions and their Current-Driven Dynamics in Ultrathin Co films

Woo S, Litzius K, Krüger B, Im M-Y, Caretta L, Richter K, Mann M, Krone A, Reeve R, Weigand M, Agrawal P, Lemesh I, Mawass M, Fischer P, Kläui M, Beach G

Magnetic skyrmions are topologically stabilized nanoscale spin configurations that show promise for future spintronic devices. However, individual skyrmions have not yet been manipulated in applications' relevant geometries. We report the observation of stable skyrmions at room temperature in ultrathin multilayer films and drive individual skyrmions by short current pulses along a magnetic wire.

8 Time-Resolved X-Ray Microscopy in Magnetic Vortex Structures: 100 ps Vortex Core Reversal and Three-Dimensional Eigenmodes

Noske M, Dieterle G, Förster J, Weigand M, Bykova Iu, Bechtel M, Stoll H, Fähnle M, Gangwar A, Woltersdorf G, Slavin A N, Back C H, Schütz G

At the MAXYMUS STXM (BL UE46) spin wave mediated 100 ps vortex core reversal was imaged as well as the three-dimensional (3D) first order gyromode. Depending on the sample thickness 3D hybridized modes exist between azimuthal spin waves and higher order gyromodes. Thus the "third dimension" has to be considered for micromagnetic simulations of vortex core reversal even at moderate thicknesses.

9 Resolving the Atmospheric Processing of Aerosols - An Environmental Chamber for X-ray Microscopy

Förster JD, Pöhlker C, Walter D, Gurk C, Kenntner T, Weigand M, Bechtel M, Andreae MO

A miniature environmental chamber for the Magnetic X-ray Microscope with UHV Spectroscopy (MAXYMUS) has been developed. It allows STXM-NEXAFS analysis in the soft X-ray region (270-2000 eV) under controlled pressure (150-1000 mbar), temperature (RT to 250 K) and humidity levels (0-95% RH), thereby extending the microscope's capabilities in the field of aerosol research and environmental science.

11 Ultrafast Magnetization Dynamics of Gd studied by XMCD in Reflection

Trabant C, Bobowski K, Frietsch B, Gleich M, Pontius N, Schüßler-Langeheine C, Wietstruk M and Weinelt M

We studied the ultrafast magnetization dynamics in single-crystalline Gd(0001) by XMCD in reflection . We find a two-step demagnetization, in agreement with former XMCD data. With increasing pump fluence the magnetization decreases exponentially in the first few ps but linear on the 100-ps time scale. For the latter we observe critical slowing down. The dynamics cannot be described by the M3TM.

15 Magnetization Dynamics in Ferromagnetic Layers Produced by Spin-polarized Current

Khan M I, Hackl J, Nemšák S, Parlak U, Doğanay H, Gottlob G, Cramm S, Bürgler D, Schneider C M

The spin-polarized current induced magnetization dynamics is investigated by time resolved X-ray PEEM. Changes in the magnetic domain pattern of the permalloy structure are observed upon the current pulse application. The pump-probe approach is then used to image the time evolution of the domain wall's magnetization by synchronizing the current pulse with the synchrotron radiation pulse train.

16 Investigating electronic transport properties of ferroelectric domains and domain walls by LEEM and X-PEEM

Schaab J, Hackl J, Khan I, Doğanay H, Gottlob D, Nemšák S, Krug I P, Schneider C M, and Meier D

We characterize conductance properties of domains and their walls in ferroic oxides in innovative LEEM and X-PEEM experiments. The electronic transport of functional domains in $SrMnO_3$ is mapped with nanoscale precision and drastically reduced acquisition times by low-energy electrons, whereas local conductance properties at ferroelectric domain walls in $ErMnO_3$ become accessible in terms of X-PEEM.

17 Surface defect chemistry of lanthanum ferrite perovskites

Mueller DN, Hackl J, Khan MI, Nemšák S, Machala ML, Bluhm H, Chueh WC, Schneider CM

The surface chemistry and morphology of lanthanum ferrites are key properties that govern the materials' performances in electrochemical applications. Using X-PEEM, we resolved surface precipitates formed after exposure to operating conditions and investigated their chemistry and thus gathered valuable insights on the surface defect chemistry and its implications for electrochemical performance.

29 Fermi level shift as an indicator of spin current induced by circularly polarized synchrotron radiation

Shevelev VO, Klimovskikh II, Vladimirov GG, Shikin AM

One of directions of spintronics investigations is creation and manipulation of spin currents. Selective photoexcitation of electrons from spin polarized opposite branches of Rashba systems may generate spin currents and be indicated as energy shift in photoelectron spectra. One of the highest known value of splitting belongs to BiTeI.

30 Graphene on cubic-SiC(001)

Aristov VYu, Molodtsova OV, Marchenko D, Sánchez-Barriga J, Mandal PS, Varykhalov A, Babenkov SV, Wu H-C, and Chaika A

Here we present the results of atomically resolved scanning tunneling microscopy, low energy electron diffraction, low energy electron microscopy and angle resolved photoelectron spectroscopy studies of graphene synthesized on cubic SiC.

32 Active optics for time resolved experiments

Vadilonga S, Zizak I, Erko A, Roshchupkin DV

A new concept of active optical devices for synchrotron radiation is presented. Surface acoustic waves create temporarily grating-like structures with amplitude up to one nanometer. The designs of X ray optical elements are discussed. It was demonstrated the synchrotron radiation modulation by a bunch-picking chopper with the time resolution better than 100 ns (tuned to BESSY II bunch structure).

33 Automated software solutions for structural biology at the HZB MX beamlines

Sparta K, Schiebel J, Huschmann F, Ühlein M, Heine A, Klebe G, Heinemann U, Weiss M S, Mueller U

XDSAPP is an expert system for automated processing of X-ray diffraction images from single crystals, based on the program suites XDS, CCP4 and PHENIX. For fragment screening experiments, an automated refinement and ligand search pipeline based on CCP4, PHENIX and COOT is being developed for use after data processing. We present the latest developments of those projects.

34 Prostate cancer protein - KDM4 - crysallographic ligand binding studies.

Malecki PH, Carter D, Muller U, Weiss M, Heinemann U, Gohlke U

Changes in histone lysine methylation pattern have been observed in cancer cells. Two isoforms of histone lysine demethylases – KDM4A and C, members of Fe2+ 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.

35 Structure Analysis of Wild-Type Human Prolidase and Its Mutations Gives Insight Into the Catalysed Reaction and Prolidase Deficiency Disease Mechanisms

Wilk P, Ühlein M, Dobbek H, Weiss MS, Mueller U

In humans prolidase is the only metalloenzyme that cleaves dipeptides containing proline residue at the C-terminus. Prolidase deficiency is a disorder manifested by various clinical symptoms. The structural basis of the enzyme inactivation are investigated. For better understanding substrate binding specificity and catalysed reaction mechanism was analysed for wild-type protein.

36 Crystallographic fragment screening: challenges, opportunities and lessons learned

Heine A, Schiebel J, Radeva N, Metz A, Huschmann FU, Ühlein M, Sparta K, Weiss MS, Mueller U, Klebe G

Fragment screening is an established method in pharmaceutical drug research. We generated a library, consisting of 361 compounds and screened it against endothiapepsin, a model system for proteins involved in serious diseases. In addition to various prescreening methods we performed a full crystallographic screening that resulted in more than 70 complex structures. Obtained hits will be discussed.

37 Structure of 17beta-Hydroxysteroid Dehydrogenase 14 with First-in-Class Inhibitors

Bertoletti N, Braun F, Möller G, Adamski J, Heine A, Klebe G, Marchais-Oberwinkler S.

17beta-Hydroxysteroid dehydrogenase14 is a recently characterized enzyme, located in the brain with a yet unclear physiological role. The enzyme catalyses the oxidation in vitro of estradiol and 5androstene-3beta,17beta-diol to estrone, dehydroepiandrosterone, with NAD+ as cofactor. The enzyme was crystallized as apo, holo structure and in complex with its substrate and our most potent inhibitors.

38 Cofactor binding to the styrene monooxygenase StyA1 requires conformational changes of the substrate binding pocket

Weiße, R H-J, Roth C, Tischler D, Sträter, N

Styrene monooxygenases are versatile catalysts facilitating epoxygenation of alkenes rendering them interesting for biotechnological applications in enantioselective synthesis. Crystals of apo styrene monooxygenase StyA1 were soaked with FAD and ADP. In the FAD complex conformational rearrangements were observed, which allowed identification of the potential substrate binding pocket.

39 Exploring unusual myxobacterial pathways- insights into the regulation of alternative isovaleryl-CoA biosynthesis

Bock T, Volz C, Müller R, Blankenfeldt W

We present the crystal structure of the transcriptional regulator AibR in the ligand free-state and bound to its possible regulator, IV-CoA. By using microscale thermophoresis (MST) we could show the specificity towards IV-CoA. With electrophoretic mobility shift assays and MST we identified the DNA binding site of AibR and showed that binding is mediated by the presence of IV-CoA.

40 Coating Bound Ligands by Tailored Water Networks to Improve Inhibitor Binding Profile for Thermolysin

Krimmer SG, Cramer J, Betz M, Heine A, Klebe G

Upon protein-ligand complex formation, water molecules arrange across the newly created surface. In a thermolysin ligand series, modified P2' substituents varied systematically the adjacent water network, correlating well with the thermodynamic signatures of complex formation. Based on these findings, we designed apolar P2' groups to improve ligand affinity and stabilize the coating water network.

41 Facilities for Macromolecular Crystallography at the HZB

Gerlach M, Förster R, Hellmig M, Huschmann F, Kastner A, Malecki P, Schmuckermaier L, Sparta K, Steffien M, Ühlein M, Weiss MS, Wilk P, Mueller U

The MX-group at the HZB operates the three beamlines BL14.1-3. With more than 1500 PDB depositions, these are the most productive MX-stations in Germany. They feature state-of-the-art experimental stations and ancillary facilities, serving 100 research groups across Europe. The BL14.2 end station has just been upgraded completely to enable automated fragment screening of up to 294 samples.

42 Frag2Xtal: Fragment screening at the MX-beamlines of the Helmholtz-Zentrum Berlin

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

The screening of target proteins with small organic molecules (termed fragments), has developed into a widely applied technique in drug development and surface mapping of proteins. A 96-fragment-library has been validated against two targets, with each revealing a hit rate of about 10%. The library is available for academic and industrial users of the HZB-MX beamlines.

43 Semi-flexible binding of cyclodextrins in a maltodextrin binding protein

Bommer M, Homburg C, Licht A, Schneider E, Dobbek H

Substrate binding proteins retrieve nutrients for ABC-importers in a dog-and-bone fashion. The structure of a maltodextrin-binding protein was solved by Sulphur-SAD. Maltotriose, maltotetraose and 6/7/8-cyclodextrin states were refined to 0.92-1.15 A. The 3-part sugar was bound tightly, while any additional sugar rings show multiple conformations and directional flexibility.

44 A guide to data collection using the beamline 14.1 Pilatus 6M detector

Bommer M, Sparta K, Dobbek H, Weiss MS, Mueller, U

While the introduction of the Pilatus 6M detector has brought automatic benefits, a few changes in data collection strategy maximise its potential. Fine phi slicing and high multiplicity benefit the isolation of anomalous scatterers, SAD phasing and high resolution data collection.

45 Structural characterisation of novel potent inhibitors for treatment of TB infections

Eltschkner S, Yu W, Pschibul A, Kisker C, Tonge PJ

Tuberculosis infections have become a life-threatening issue during the last years. For that reason new and effective antibiotics are urgently needed. Novel diaryl ether compounds were designed, aiming to prolong the residence time in InhA, a fatty acid synthesis II enzyme of Mycobacterium tuberculosis.

46 Monitoring the post-synthetic functionalization of MOFs by synchrotron single crystal X-ray diffraction

Müller P, Wisser FM, Bon V, Grünker R, Senkovska I, Kaskel S

A series of highly porous crystalline materials for vapochromic sensing of alcohols was designed by post-synthetic paddle-wheel crosslinking and functionalization of 1,3-phenylenebis(azanetriyl)tetrabenzoate based MOFs. The crystal structures of MOFs, containing up to 76.2 % of disordered solvent in the pores, could be unambiguously determined using datasets collected on the MX BL14.2 beamline.

50 Joint Analysis of Radiative and Non-radiative Electronic Relaxation Upon X-ray Irradiation of Transition Metal Aqueous Solutions

Golnak R, Bokarev SI, Seidel R, Xiao J, Grell G, Atak K, Unger I, Thürmer S, Aziz SG, Kühn O, Winter B, Aziz EF

XAS is often probed in the total or partial fluorescence yield modes, what leads to inherent distortions with respect to the true transmission spectrum. By applying both photon- and electron-yield techniques together with high-level first principles calculations we demonstrate that partial yield arising from the 3s to 2p relaxation is a more reliable probe of XAS than the 3d to 2p one.

51 Determination of the Electronic Structure of Aqueous Urea and its Derivatives: A combined Soft X-Ray – TD-DFT Approach

Tesch MF, Golnak R, Ehrhard F, Schön D, Xiao J, Bande A, Aziz EF

We present soft x-ray absorption, emission and resonant inelastic scattering measurements at the nitrogen K-edges of urea and selected derivatives dissolved in water. We show that it is crucial to consider the localized nature of the x-ray interaction at the N sites of the molecules and compare the experimental spectra to TD-DFT calculations to extract overall molecular properties like the chemical relevant HOMO-LUMO gap from the measurements.

52 Strong correlated electronic system in Mn3+ oxide revealed by RIXS

Schön D, Xiao M, Golnak R, Tesch MF, Aziz EF

MnO_x has been demonstrated as effective water oxidation catalysts, among which Mn3+ species is proven as the most efficient ingredient when compared to other Mn oxidation states. We selected Mnacac3 in dichloromethane as a prototypic system to carry out in-situ RIXS measurements. Intense RIXS loss features are observed, implying a highly localized and strong correlated system in d4 configuration.

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

Seidel R, Pohl M, 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.

54 Surface reactions of CO and C2H4 on carbide-modified Mo(110)

Bauer U, Gleichweit C, Späth F, Höfert O, Steinrück H-P, Papp C

We investigated the reactions of CO and C_2H_4 on carbide-modified Mo(110) as a noble metal-free catalyst using TPXPS, NEXAFS and TPD. Upon CO adsorption, we detect several species and partial dissociation. During heating, most CO desorbs molecularly up to 460 K. At 800 K recombinative desorption of C and O is observed. C_2H_4 adsorbs tilted and dehydrogenates via an ethylidyne intermediate.

55 Reactivity of hexagonal Boron Nitride on Nickel towards atomic hydrogen

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

We report on the hydrogenation and dehydrogenation of hexagonal Boron Nitride prepared on a Ni(111) single crystal. We adsorb atomic hydrogen at low temperatures, and study the system subsequently with synchrotron based temperature programmed photoelectron spectroscopy, temperature programmed desorption, near edge adsorption fine structure and ultraviolet photoelectron spectroscopy.

56 Towards a fundamental understanding of practical ionic interfaces: PES adsorption studies on lithium-ion electrode materials

Fingerle M, Späth T, Schultz N, Hausbrand R

Ionic interfaces play a key role for the performance of electrochemical devices. Here, a surface science approach to improve the fundamental understanding with respect to reactivity and charge transfer is presented. Interfaces of thin film lithium-ion insertion material with different adsorbate species are prepared step-by-step and the evolution of the surface electronic structure with coverage is monitored by PES and used to establish energy level diagrams.

57 Al and Ag nanoparticles in $CuPcF_4$ organic film

Molodtsova OV, Aristova IM, Babenkov SV, Vyalikh DV, Vilkov OV, and VYu Aristov,

The evolution of the morphology and the electronic properties of the hybrid organic-inorganic systems composed of aluminum and silver nanoparticles distributed in an organic matrix tetrafluoro copper phthalocyanine, as a function of nominal metal content was studied by transmission electron microscopy and by surface and bulk sensitive photoelectron spectroscopy.

58 Self assembled gold nanoparticles in $CuPcF_4$ molecular crystal

Babenkov SV, Molodtsova OV, Aristova IM, Tchaplyguine M, and Aristov VYu

The evolution of the morphology and the electronic properties of the hybrid organic-inorganic systems composed of gold nanoparticles distributed in an organic matrix tetrafluoro copper phthalocyanine, as a function of nominal Au content was studied by transmission electron microscopy and by surface and bulk sensitive photoelectron spectroscopy.

58a Morphology of metallic nanoparticles self organized in CuPc film

Aristova IM, Babenkov SV, Molodtsova OV, Vyalikh DV, Vilkov OV, and Aristov VYu

The evolution of the morphology and the electronic properties of the hybrid organic-inorganic systems composed of aluminum, silver and gold nanoparticles distributed in an organic matrix, copper phthalocyanine as a function of nominal metal content was studied by transmission electron microscopy and by surface- and bulk sensitive photoelectron spectroscopy.

59 Synchrotron-based Mid-infrared Single-shot Spectrometer

Ritter E, Puskar L, Hofmann KP, Aziz EF, Hegemann P, Schade U

A novel infrared ‘Single-shot’-spectrometer for measuring irreversible reactions with microsecond time-resolution is shown. It is based on a dispersive approach with a modern focal plane array detector. Together with IR-synchrotron light, the unique optical concept allows a high S/N in single-shot mode. First spectra obtained with a conventional globar source proof the aimed design parameters.

60 FTIR spectroscopy view of the proton exchange membrane (PEM) dynamics.

Puskar L, Ritter E, Aziz EF, Schade U

Light-driven water oxidation is a vital step in harvesting the solar energy. Catalysts oxidising water at potentials close to thermodynamic limit are of special interest. The high proton conductivity and stability of ionomer membranes (PEM) makes them popular for catalyst immobilization inside fuel cells. FTIR was applied to investigate the nature of interactions in multi acid side-chain ionomers.

61 An XUV At-Wavelength Metrology facility at BESSY-II

Sokolov A, Bischoff P, Eggenstein F, Erko A, Gaupp A, Künstner S, Mast M, Schmidt J-S, Senf F, Siewert F, Zeschke Th, Schäfers F

The novel powerful metrology facility with new Optics Beamline and a Reflectometer has gone into operation for at-wavelength characterization and calibration of the in-house produced gratings and novel nano-optical devices as well as mirrors, multilayered systems etc. It is now opened for all user. First results on optical performance and measurements on multilayer grating and will be presented.

63 Al diffusion and initial oxidation in FeAl and FeCrAl alloys

Granroth S, Perälä R, Heinonen M, Kilpi T, Kukk E, McLaren I, Andertsson S, Kokko K

Hard X-ray Photoelectron Spectroscopy (HAXPES) and Transmission Electron Microscopy (TEM) were used to investigate the initial oxidation of FeAl and FeCrAl alloys and the effect of Cr on the segregation of Al (third element effect). Photoemission experiments were carried out at KMC-1 beamline using HIKE end-station.

64 Enhanced ferrimagnetism in auxetic $NiFe_2O_4$ in the crossover to the ultrathin-film limit

Hoppe M, Döring S, Gorgoi M, Cramm S, and Müller M

We explore the enhanced magnetic properties of single-crystalline $NiFe_2O_4$ films from bulk to ultrathin films. We performed a complementing spectroscopic analysis employing bulk- and surface-sensitive photon spectroscopies (HAXPES, XANES, XMCD). Determining the element-specific valencies and coordinations reveals the absence of any cation inversion, as was held respnsible for enhanced MS.

65 Investigation of the potassium fluoride post deposition treatment on the CIGSe/CdS interface using hard x-ray photoemission spectroscopy-a comparative study

Ümsür B, Calvet W, Steigert A, Lauermann I, Gorgoi M, Prietzel K, Greiner D, Kaufmann CA, Unold T, Lux-Steiner MCh

We investigated the influence of KF-post deposition treatment (PDT) on CIGS/CdS interface using HAXPES. We found that the surface near Cu and Ga concentrations are lower on the KF-treated sample. The depth dependent onset of the CIGS valence band in contact to CdS is shifted to lower binding energies on the KF-PDT CIGS/CdS layer system.

66 Magnetophotoresistance in $Pr_{(0.6)}Ca_{(0.4)}MnO_3$ thin film

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

The colossal magnetoresistive insulator to metal switching of almost nine orders of magnitude under the significantly reduced magnetic field is achieved by illumination for the low bandwidth manganite $Pr_{(0.6)}Ca_{(0.4)}MnO_3$ thin film at low temperatures. The high kinetic energy XPS measurements at 300 and 120 K temperatures are made for this material.

66a Compound and interface formation of mixed halide perovskites

Handick E, Sadoughi G, Starr D. E, Wilks R. G, Alsmeier J.-H, Köhler L, Gorgoi M, Félix R, Snaith H, and Bär M

Recent breakthroughs of hybrid organic-inorganic perovskite solar cells have demonstrated their high potential. HAXPES at BESSY II (HiKE at KMC-1) was used to in-situ study the compound formation and to monitor the interface formation of $CH_3NH_3PbI_{3-x}Cl_x$ on compact and mesoporous TiO_2. We find that annealing temperature and substrate have a pronounced impact on compound and interface formation.

67 Nanoscale defects in Sr_2FeMoO_6 thin films

Saloaro M, Granroth S, Hoffmann M, Adeagbo W A, Deniz H, Palonen H, Huhtinen H, Majumdar S, Laukkanen P, Hergert W, Ernst A and Paturi P

The nanoscale defects have proven to be an important factor in Sr_2FeMoO_6 thin films, which have excellent properties for spintronic applications. Therefore, we have investigated the effect of lattice mismatch, anti-site disorder and oxygen vacancies with theoretical calculations and various experiments. The experimental studies were made with HAXPES (HIKE, KMC-1), XRD, TEM and SQUID magnetometer.

68 Chemical states of nanocrystalline CoS_2 pre- and post-operation in a PV-device studied with HAXPES

Johansson F, Fondell M, Lindblad A

Nanocrystalline CoS_2 grown on reduced graphene oxide has been studied as a counter electrode in a dye-sensitized solar cell as an alternative to platinum. Using HAXPES we show that contact with the electrolyte and operation cleans the starting material and induces new chemical states in the utility material whiles leaves the rGO network intact. The new chemical state is a substoichiometric CoS_2.

69 Attosecond charge transfer in 2H-MoS_2

Johansson F, Fondell M, Lindblad A.

The charge transfer time (CTt) in single crystal MoS_2 have been studied with the core-hole clock method in the region of the S KLL Auger final state with two holes in the S 2p and the resonant Auger final state with two holes in the S 2p and one electron in states hybridized with the S 3p orbital in the conduction band. We demonstrate a CTt of 300 attoseconds.

70 Monitoring the interface formation in thin-film solar cells by hard x-ray photoelectron spectroscopy

Köhler L, Yang P, Brandt RE, Reinhard P, Bissig B, Avancini E, Yang C, Handick E, Hartmann C, Liao X, Kunze T, Félix R, Wilks RG, Gordon RG, Buecheler S, Tiwari AN, Buonassisi T, Bär M

The interface formation in thin-film solar cell devices was studied by HAXPES at the HiKE endstation (BESSY II KMC-1 beamline). Our results on the interface structure of (a) the ZnO/SnS and (b) the CdS/Cu(In,Ga)Se_2 layer stack are presented. We gain insight on how (a) the surface oxidation of SnS and (b) different alkali postdeposition treatments of Cu(In,Ga)Se_2 affect the interface structure.

71 Single-shot XAFS at the BAMline - new analytical possibilities for in situ material characterization.

Guilherme Buzanich A, Radtke M, Reinholz U, Riesemeier H

A concept that entails both time and lateral resolution simultaneously in one shot to perform XANES measurements is presented. Being this of extreme importance in several fields, it is particular interesting for the field of catalysis, especially in the case of chemically heterogeneous catalysts by in situ / operando approaches.

72 CO adsorption on EuroPt-1 studied with a new in-situ XAS-DRIFTS cell

Brieger C, Melke J, Roth C

T-dependent CO desorption has been studied on EuroPt-1 (6.3 wt. % Pt/SiO2). Using our new in-situ XAS-DRIFTS cell we can monitor bulk and surface adsorbates simultaneously. From 25-150°C we observe CO at the surface (DRIFTS) while the bulk adsorbates shift from CO to an O-species (delta μ XANES). EXAFS data give hints for reconstruction of the nanoparticles which are interpreted as SMSI.

73 IN-OPERANDO CHARACTERISATION OF PEMFCS USING SYNCHROTRON X-RAY RADIOGRAPHY AND TOMOGRAPHY

AIrwashdeh S, Markötter H, Arlt T, Haußmann J, Klages M, Scholta J, Riesemeier H, Müller B, Kupsch A, Manke I, Banhart J

Water transport in PEMFCs is investigated by synchrotron X-ray imaging. Three different techniques are described on this poster, namely Tomography, in-plane and through-plane radiography that yield information on the water distribution in the cell materials. It is shown how the water distribution and transport is quantified and visualized.

74 3D Microstructure Characterization of Al MMC by means of Synchrotron Micro-Tomography at BAMline-BESSY II

Mishurova T, Cabeza S, Léonard F, Staude A, Bruno G

Synchrotron radiation and absorption tomography were employed to characterize aluminum three and four phase composites Al_{12}SiNiCuMg 15 Al_2O_3 and Al_{12}SiNiCuMg 7 Al_2O_3 15 SiC, with a preferential orientation of reinforcement within a plane. The analysis of 3D microstructure disclosed the distribution and volume fraction of the different phases, as well as their evolution after thermal treatment.

75 SYNCHROTRON X-RAY IMAGING FOR CHARACTERIZATION OF FUEL CELL MATERIALS

Markötter H, Haußmann J, Klages M, Seidenberger K, Wilhelm F, Krüger P, 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. Additionally the role of cracks in the microporous layer is demonstrated.

76 Performance optimization of phase grating in parallel beam for grating interferometry

Shashev Y, Kupsch A, Lange A, Müller BR, Bruno G, Hentschel MP, Britzke R

We examined the visibility of phase gratings by varying different geometric parameters. Rotation about the vertical axis changes the distribution of phase shifts and yields higher visibility than for normal grating alignment. Tilting the grating in the scattering plane enables a continuously varying grating height. This opens the way to adjust the photon energy suited for the respective materials.

77 3D Imaging of Hydrogen Assisted Cracking using Analyser-Based Imaging

Laquai R, Schaupp T, Müller BR, Griesche A, Bruno G, Kannengiesser T

Hydrogen in metals can cause a degradation of the mechanical properties. In combination with internal stresses hydrogen assisted cracking can occur. To better understand this phenomenon we used Analyser-Based Imaging combined with CT to image the 3D distribution of the internal interface density in an EN AW-6060 weld. By employing this method more details of the crack network could be identified.

78 Formation of refractive distortions in radiology

Evsevleev S, Hentschel MP, Lange A, Kupsch A, Müller BR

We demonstrate the formation of the so-called X-ray phase contrast at simply shaped bodies. Measurements exhibit intensity pile-up as well as pronounced minima. A thorough comparison to simulations based on pure ray optics (Snell's law) and wave optics (Huygens wave propagation) showed excellent agreement.

79 Time resolved studies on the formation mechanism of iron oxide nanoparticles using combined fast-XANES and SAXS

Kabelitz A, Guilherme A, Reinholz U, Radtke M, Bienert R, Schulz K, Krähnert R, Emmerling F

In the present contribution, we report on the in situ investigation of an iron oxide nanoparticle synthesis by coupled X-ray absorption near-edge structure (XANES) and Small Angle X-ray Scattering (SAXS). The combination provides simultaneously information about the size and shape of particles (SAXS) and on the oxidation state and the local structure of the iron atoms (XANES).

80 Biomineral characterization using small and wide angle X-ray scattering at the BESSY II µSpot beamline

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

The unique combination of simultaneous microbeam scanning SAXS/WAXS together with XRF or RAMAN at the BESSY II µSpot beamline allows the characterization of structure and composition of (i) diseased bone material, (ii) changes in polymer-metalfluoride particle composites during in-situ tensile testing and of (iii) crystallized calcium carbonate microlens arrays.

81 Paracetamol: Polymorphs and Intermediates

Nguyen Thi Y, Rademann K, Emmerling F

In situ studies of WAXS and Raman spectroscopy enable the monitoring of crystallization processes from solution via amorphous phases to stable crystalline forms. Diffuse scattering from amorphous intermediates analyzed by using atomic pair distribution function was determined. The influence of different solvents on the crystallization of paracetamol was investigated using an acoustic levitator.

82 Electronic structure of thionized diamondoids

Zimmermann T, Höhne T, Knecht A, Richter R, Fokin AA, Schreiner PR, Möller T, Rander T

The optical properties of diamondoids, perfectly size- and shape-selectable sp^3-hybridized carbon nanoparticles, are expected to be drastically modified upon sulfurization. We investigated the UV absorption cross section of various sized thionized diamondoids at the U125-2 10m-NIM beamline and could determine strong shifts of optical gaps in comparison to their corresponding pristine analogues.

90 Electronic properties of In and Sn/In2O3 interfaces

Nazarzadehmoafi M, Siebert A, Titze F, Janowitz C, Galazka Z, Manzke R, and Mulazzi M

To shed light on the microscopic origin of the conduction in In_2O_3, the behavior of the electronic structure of melt-grown In_2O_3 (111) single crystals was studied upon In and Sn deposition using angle-resolved photoemission spectroscopy. Both interfaces show ohmic behavior. The initial stage of In growth on In_2O_3 was accompanied by formation of a 2DEG, while it was not observed by Sn coverage.

99 The Electronic Structure of Iridium Oxide Electrodes Active in Water Splitting

Pfeifer V, Jones T E, Velasco-Vélez J J, Massué C, Scherzer M, Arrigo R, Hävecker M, Knop-Gericke A, Schlögl R

We investigate OER-active IrO_x surface species by XPS and NEXAFS. Compared to less active rutile IrO_2, amorphous IrO_x shows a pre-edge feature in the O K-edge caused by O 2p hole states and additional intensity at higher BEs in the Ir 4f spectrum attributed to Ir^{3+} species. These electronic defects in the anionic and cationic framework of IrO_x are likely critical for its enhanced OER-activity.

100 The electronic structure of Tb silicide nanowires and thin films on Si surfaces

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

The electronic properties of Tb silicide nanowires and thin films grown by self-organisation on Si surfaces with various orientations are analysed using XPS and ARPES. Flat band conditions are observed for all structures on n-type samples. Their electronic dimensionality illustrated by their Fermi surface varies strongly and will be discussed in the context of their structure derived by STM.

101 Molecular Interlayer Mediated Potassium Doping of Graphene

Raidel C, Göhler F, Guo J, Speck F, Dzhagan V, Zahn DRT, Seyller T, Wanke M

We report on the adsorption doping of graphene on 6H SiC(0001) with Mn-Phthalocyanine (MnPc) and subsequent doping with potassium. ARPES and XPS were used to determine the charge transfer from MnPc to graphene, while NEXAFS was used to determine the orientation of the molecule. Subsequent potassium deposition leads to a charge transfer from the potassium to the MnPc and therefore to the graphene.

102 The MAXYMUS X-ray Microscope: An Overview

Weigand M, Bykova I, Bechtel M, Goering E, Van Waeyenberge B, Schütz G

The MAXYMUS scanning soft X-ray microscope is a permanent endstation at the UE46-PGM2 beamline with special focus on magnetic and time resolved microscope. We will present an overview of the capabilities of the microscope, highlighting recent developments including sample cryo stages cooling, ultra-high resolution ptychographic imaging and the use of low-alpha mode for fast dynamic acquisitions.

103 Light-induced ring-closure isomerization of diarylethene molecules adsorbed on solid surfaces

Nickel F, Bernien M, Wrzalek S, Herder M, Chittas P, Kraffert K, Arruda L M, Kipgen L, Hecht S, Kuch W

Grafting photochromic diarylethene molecules on a solid surface is of great interest for the field of molecular electronics because of the conjugated conduction path in the closed-form isomer. We compare the light-induced ring-closure of diarylethene molecules, consisting of thiazol moieties, adsorbed on Au(111), Bi(111), and HOPG surfaces, studied by NEXAFS, XPS, and DFT simulations.

104 Higher Order Corrected Spectroscopy at the Carbon K Edge

Jansing C, Mertins H-C, Gaupp A, Sokolov A, Gilbert M, Schümmer A, Wahab H, Timmers H

Synchrotron X-ray experiments inevitably contaminate optical beamline elements. Consequently, at the carbon K edge, absorption can drastically reduce photon flux, so that incident light has large contributions from higher order wavelengths. The efficacy of a correction method is demonstrated. The novel procedure permits reliable spectroscopy of carbonaceous materials such as HOPG or graphene.

105 decay in aqueous solution as a unique probe of ion pairing and structure

Pohl M, Seidel R, Unger I, Aziz EF, Winter B, 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.

106 PEAXIS at BESSY II: Design of the new Endstation for RIXS and XPS Measurements and Potential Applications

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

We present a new endstation for Photo Electron Analysis and X-ray resonant Inelastic Spectroscopy (PEAXIS) at BESSY II. Its expected performance is shown by means of ray tracing simulation. Additionally, potential applications like element-specific and momentum-resolved studies on elementary (for instance electronic) excitations in thermoelectrics and catalysts for energy conversion are discussed.

115 Investigations on isolated Single Molecule Magnets by X-ray Magnetic Circular Dichroism spectroscopy

Hewer J, Tombers M, Lang J, Niedner-Schatteburg G, Bülow C, Lau T

We utilized XMCD spectroscopy in the gas phase to investigate the intrinsic magnetic properties of different SMM of the $[Mn_2LnLx]+$ -type Ln: Nd/Eu/Gd/Dy/Lu. Gas phase investigations allow for a magnetic characterization of these SMMs void of any surface or packing effects. The selectivity of the XMCD technique allows us to determine the contribution of the different metals to the magnetic moment.

116 XMCD Spectroscopy of Free Transition Metal Atomic Ions: Fundamental Test of Sum Rules for 3d Elements

Leistner G, Zamudio-Bayer V, Bülow C, Lindblad R, Ławicki A, Hirsch K, Terasaki A, von Issendorff B, Lau JT

Sum rules for XMCD spectroscopy have been derived more than 20 years ago, but have never been tested on truly atomic systems. We present the first XMCD spectra of free iron, cobalt, and nickel atomic cations, recorded in a magnetic field of 5 T at 15-20 K ion temperature in a linear ion trap. We will discuss the validity of XMCD sum rules and the magnitude and sign of the magnetic dipole term.

117 Magnetic properties of free hydrogenated manganese-doped silicon clusters

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

The magnetic moment of $MnSi_n$ clusters is quenched for n > 10. DFT predicts a restoration of the moment by hydrogen passivation. By XMCD and XAS measurements we show that the magnetic properties of $MnSi_n$ clusters change significantly by hydrogen passivation. While the sizes n = 10 - 14 carry a magnetic moment, the moment of n = 16 is again quenched, possibly due to a structural change.

118 X-ray magnetic circular dichroism spectroscopy of 3d transition metal diatomic molecules in the gas phase

Zamudio-Bayer V, Hirsch K, Langenberg A, Ławicki A, Lindblad R, Bülow C, Leistner G, Terasaki A, von Issendorff B, Lau T

Despite their trivial geometry and stoichiometry, homonuclear diatomic 3d transition metal molecules have a complex electronic structure. Its theoretical description remains challenging up to now. We have experimentally resolved the spin and orbital magnetic moment contributions to the ground state of Cr, Mn, Fe, Co, and Ni dimers and find unpredicted high spin states or orbital magnetic moments.

119 The new Coincidence-ESCA station at BESSY II

Leitner T, Ovsyannikov R, Sassa Y, Zhang T, Bidermane I, Mucke M, Gorgoi M, Föhlisch A, Svensson S, Mårtensson N

We introduce the new CoESCA station, which will be available for user operation in the second semester of 2016. The experimental station will be equipped with two ArTOF spectrometers and a state-of-the-art UHV manipulation and sample preparation system, in order to enable (angular-resolved) electron-electron coincidence spectroscopy on solid materials and their surfaces.

120 Near Edge X-ray Absorption Fine Structure Spectroscopy of Free Iron Oxide Nanoparticles

Langer B, Goroncy C, Raschpichler C, Fortscher J, Antonsson E, Graf C, Rühl E

We report X-ray absorption measurements of free iron oxide nanoparticles (d=10-40 nm) in a particle beam near the Fe 2p edge as a function of the nanoparticle size with and without post-synthesis oxidation. The absorption spectra show distinct near edge structures that can be assigned to magnetite or maghemite, with the ratio varying as a function of particle size and post synthesis oxidation.

121 Angular Distributions from LiquidWater: Effects of Electron Scattering

Seidel R, Unger I, Pohl M, Bradforth S, Tobias D, Thürmer S, Abel B, Siefermann K, Hergenhahn U, Aziz EF, Winter B

Liquid-microjet X-ray photoelectron (PE) spectroscopy measurements from aqueous salt solutions were performed to quantify electron probing depth into solution. By measuring O1s PE spectra at different linear polarizations and a wide range of photon energies we explored how the presence of a surface monolayer or the presence of Na+ and I- scattering centers modify the O1s PAD from neat water.

122 Sample Environments for Synchrotron Radiation Experiments

Klemke B, Grimm N, Gerischer S, Wallacher D, Kiefer K

Ionic interfaces play a key role for the performance of electrochemical devices. Here, a surface science approach to improve the fundamental understanding with respect to reactivity and charge transfer is presented. Interfaces of thin film lithium-ion insertion material with different adsorbate species are prepared step-by-step and the evolution of the surface electronic structure with coverage is monitored by PES and used to establish energy level diagrams.

123 Parallelized gas adsorption and synchrotron powder X-ray diffraction / EXAFS on switchable MOFs

Bon V, Krause S, Senkovska I, Wallacher D, Többens DM, Zander S, Kaskel S

A unique combination of EXAFS and powder XRD with gas adsorption experiments, performed at the KMC-2 beamline, shed light on the negative gas adsorption phenomenon in the pressure amplifying framework DUT-49(Cu), possessing hierarchical pore structure. To the best of our knowledge, pressure amplifying materials of this magnitude have never been reported before.

124 Anomalous X-ray diffraction study of Cu2ZnSn(S1-xSex)4 (CZTSSe)

Gurieva G, Többens DM, Schorr S

CZTSSe is potential candidate for photovoltaic applications. Single phase samples were grown by solid state reaction of the elements. Anomalous X-ray powder diffraction experiments were performed using the diffraction end station of the KMC-2 beamline. Structural parameters and cation distribution were determined by Rietveld analysis of the data, providing an insight into point defects in CZTSSe.

125 Chloride Substituted Hybrid Perovskites MAPbI3-xClx - a systematic, crystallographic study

Steckhan J, Franz A, Többens D and Schorr S

The hybrid perovskite $MAPbI_3$ (MA-Methylammonium) is a promising material for thin film solar cells. Its constituents can be substituted by different elements, e. g. the addition of chloride leads to improved optoelectronic properties. Nevertheless the role of chloride is still not solved conclusively. Therefore different $MAPbI_{3-x}Cl_x$ products were examined by synchrotron X-ray diffraction.

126 Synthesis of Cu_2ZnSnS_4 (CZTS) powder via nanoparticle inks and its intrinsic point defect characterization

Diestel L, Zander S, Gu E, Franz A, Schorr S

CZTS nanocrystals, synthesized by hot injection and post-annealed, where investigated by anomalous X-ray diffraction (KMC-2) and neutron powder diffraction (E9) to gain structural informations concerning especially Cu-Zn disorder. The results of this complementary study showed significant Cu-Zn disorder on the structural sites 2c and 2d, which is comparable to this effect obtained in bulk CZTS.

127 Investigation of Local Structural Changes and Li Reaction Mechanism of Nanocrystalline $NiFe_2O_4$ by X-ray Absorption Spectroscopy

Zhou D, Permien S, Rana J, Schumacher G, Zander S, Banhart J, Bensch W

XAS is used to investigate local structural changes of $NiFe_2O_4$ anode materials during 1st cycle. At initial discharging, the spinel structure transforms to rock salt monoxide phase. Metallic products are formed at the end of discharging with a small particle size and highly disorder. All these ultrafine metal particles are reoxidized to Fe_2O_3 and NiO phase during following charging.

128 Thermal dependence of Cu/Zn ordering in CZTSe kesterites by anomalous diffraction

Többens DM, Gurieva G, Schorr S

We demonstrate by means of direct determination of the site occupancies from anomalous X-ray powder diffraction data taken at KMC-2 at the Cu- and Zn absorption edges the ordering of Cu^+ and Zn^{2+} in B-type $Cu_2ZnSnSe_4$ (CZTSe) kesterite upon annealing at temperatures below 180°C.

129 Grazing incidence x-ray diffraction from ferroelectric domains in MOCVD grown (K,Na)NbO_3 epitaxial layers

Schmidbauer M, Schwarzkopf J, Feldt C, Kwasniewski A, Braun D

Ferroelectric (K,Na)NbO_3 epitaxial layers grown by metal-organic vapor-phase deposition on (110) $NdScO_3$ substrate were investigated by grazing incidence x-ray diffraction. Owing to the specific monoclinic symmetry of the film unit cell a periodic domain pattern is formed. The morphology of the domain pattern and the in-plane monoclinic angle are evaluated as a function of layer thickness.

132 Improved Peak Fit Procedure of XPS Measurements of Inhomogeneous Samples - Development of the Advanced Tougaard Background Method

Hesse R, Weiß M, Szargan R, Streubel P, Denecke R

A new method for the fitting of x-ray photoelectron spectra using an advanced Tougaard background model for laterally inhomogeneous samples is presented. New is the use of a separate loss function for each spectral component. The new source code of the UNIFIT software (Version 2016 or higher) to calculate the advanced Tougaard-background parameters for inhomogeneous samples was verified.

133 High-resolution and stroboscopic XRPD

Schökel A, Berghäuser A, Etter M, Gorfman S, Knapp M, Hinterstein M

The improved high-resolution multi analyzer crystal detector at the P02.1 powder diffraction beamline at PETRA III (DESY) is presented. Using a FPGA based data acquisition system stroboscopic measurements with 0.00025 degree angular and 10 ns temporal resolution are possible. Recent data of a piezo ceramic sample under excitation by an electric field illustrates the capability of the system.

173 A Detailed Assignment of NEXAFS Resonances of Ionic Liquids

Ehlert C, Holzweber M, Lippitz A, Unger WES, Saalfrank P

A combination of measurements and quantum chemical calculations of C K and N K NEXAFS resonances is presented, for two kinds of imidazolium based ionic liquids ([CnC1im][NTf2] and [C4C1im][I]) . The simulations reproduce all characteristic features observed by the experiment. A detailed assignment of resonance features to excitation centers leads to a consistent interpretation of the spectra.

174 Photoemission and XANES study of doped oxide and fluoride graphite after pressure and temperature treatment

Asanov IP, Fedoseeva YV, Asanova TI, Palyanov YN, Kanygin MA, Okotrub AV, Nefedov A

Doping of graphene with different elements enhances performance of graphene-based supercapacitors. PES and XANES studies showed that pressure and temperature treatment of graphite oxide with sulfur or triphenylphosphine at 1000 C and 500 bar brings about the formation of chemical bond between sulfur or phosphor with high-crystalline graphene layers. Concentration of P and S are 1-2 at %.

175 Insight into the electronic structure of extended aromatic molecules: comparison of experimental and computational NEXAFS signatures

Klues M, Breuer T, Jerabek P, Berger R, Witte G

Combining experimental and computational NEXAFS studies provides detailed insight into the electronic nature of molecular systems which is illustrated using two examples. For the case of perfluoropentacene it explains the origin of dichroism of the F1s-NEXAFS signature while for pentacenequinone it illustrates the concept and limitation of electronic subunits.

176 Formation of Surface Amino Groups and their Application in Click Chemistry: A Silane-Free Functionalization Strategy of Silicon Nitride

Lange N, Dietrich P M, Lippitz A, Kulak N, Unger WES

In this contribution we propose a functionalization strategy of silicon nitride using SiNHx bonds. Azide-terminated surfaces were obtained from freshly prepared surface amino groups. The latter ones were generated by fluoride etching. Alkyne-terminated test molecules were then immobilized by click chemistry. Angle resolved XPS and NEXAFS were carried out at the HE-SGM beamline.

177 The influence of the rotaxane-design to the occurring of coupled molecular switching processes in ordered coordination oligomers

Heinrich T, Traulsen CH-H, Holzweber M, Dib B, Unger WES, Schalley CA

In a recent study, we showed how important it is to have densely packed as well as an ordered template for a coupled molecular switching to occur. In this work, we want to show how the rotaxane-design influences the structure of the deposited rotaxane-multilayers before and after the stimulus-induced axle-movement. We compare three different rotaxanes with different sizes and flexibilities.

178 N_2O to N_2 conversion on reduced ceria surface: NEXAFS and IRRAS studies

Nefedov A, Yang C, Wöll C

Ceria has proven to be a highly active catalyst for NO_x reduction. To monitor the conversion the NEXAFS and IRRA spectroscopies have been applied in a time-resolved fashion. Two observed resonances decrease in parallel over time and this decrease is explained by conversion of N_2O to N_2. IRRAS data confirm NEXAFS results.

179 Adsorption and desorption of water on protein-repelling self-assembled monolayers

Sayin M, Nefedov A, Zharnikov M

We studied kinetics and thermodynamics of water adsorption and desorption as well as wetting and nucleation behaviors of water on model organic surfaces, formed by OEG- SAMs. Varying the water coverage and the capability of surface hydration, we monitored transfer from the hydration to wetting regime, distinguishing between the hydration and interfacial phases and deriving their parameters.

180 Investigation of NEXAFS Resonances of Self-Assembled Monolayers by Transition Potential Density Functional Theory

Ehlert C, Unger WES, Saalfrank P

DFT has proven its power to predict NEXAFS resonances in several studies . The calculated dipole transition matrix elements can be used to interpret polarized and angle-dependent NEXAFS spectra, which holds useful information about molecular orientations. Recent results of angle-dependent NEXAFS simulations of model systems for pyridine terminated self-assembled monolayers are presented.

185 Observation of higher order Yoneda bands from lamellar gratings in GISAXS

Soltwisch V, Wernecke J, Haase A, Fernandez Herrero A, Krumrey M, Probst J, Schoengen M, Burger S and Scholze F.

X-ray scattering is a fast, non-destructive method capable of sub-nm resolution. Besides the well known diffraction peaks used for the profile reconstruction, characteristic diffuse scatter contributions from periodic nanostructures are observed in grazing incidence small angle X-ray scattering (GISAXS). The understanding of these processes opens new ways to obtain structural information.

186 X-ray absorption fine structure of sulfur in a Li-S battery cathode measured under protective atmosphere

Zech C, Müller M, Choudhury S, Beckhoff B

Lithium Sulfur (Li-S) batteries are promising candidates for improved high capacity batteries. The cycling stability of currently developed Li-S batteries is limited due to undesired side reactions. Therefore the cathode has been characterized by electrochemical cycling (functionality) and by X-ray absorption spectroscopy (material properties) under inert argon atmospheric conditions.

187 Transition probabilities of the titanium L3 fluorescence lines as a function of the oxidation state

Unterumsberger R, Müller M, Beckhoff B

The increase of the sensitivity of a wavelength-dispersive spectrometer in the soft X-ray range enables the access to high resolved X-ray emission spectrometry at nanoscaled materials. The increase could be achieved by using a single bounce monocapillary. The transition probabilities of the titanium L3 fluorescence lines were determined with low uncertainties as a function of the oxidation state.

190 Measuring Nanostructures without Breaking them: X-Ray Scattering for Nanometrology

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

For non-destructive quality control of nanostructured surfaces, Grazing Incidence Small-Angle X-Ray Scattering (GISAXS) is a promising technique. I compare GISAXS measurements of large-area (1mm x 15 mm) and small-area (down to 4µm x 4µm) patches of silicon line gratings and compare the results to simulation and complementary methods.

191 Interface properties of Mo/Si and Cr/Sc multilayer mirrors

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

We characterize high-reflectance Mo/Si and Cr/Sc multilayers with with respect to interface roughness using EUV light. The analysis of diffusely scattered light provides information on vertical and lateral correlations of roughness. In order to extract the power spectral density accurate modelling based on data from complementary experimental methods is required.

192 Characterization of optical material parameters for EUV Lithography applications at PTB

Laubis C, Haase A, Soltwisch V, Scholze F

Progress in EUV Lithography is based on new materials and R&D requires data on the optical properties of the materials involved. The required data is not readily available from databases. PTB operates instrumentation in the EUV and adjacent wavelength ranges and can provide the data for the determination of optical material parameters for individual thin layers.

193 Nanoparticle characterization by continuous contrast variation in SAXS with a solvent density gradient

Garcia-Diez R, Gollwitzer C, Krumrey M

A novel approach to contrast variation with SAXS is presented based on the constitution of a solvent density gradient in a glass capillary. SAXS curves were continuously recorded at different solvent contrasts at the four-crystal monochromator beamline of PTB. The density and size distribution of the particles were simultaneously determined and validated with an inter-laboratory comparison.

194 Synchrotron Light Probing the Liquid Solid Interface for Immobilized Biomolecules

Nutsch A, Streeck C, Weser J, Beckhoff B, Grötzsch D, Malzer W, Dietrich P, Fischer T, Nietzold C, Rurack K and Unger W

In life science the application of reference free metrology, as presented in this contribution, could be rarely found. TXRF using soft X-rays was successfully implemented for the quantification of functionalized glass slides. NEXAFS based on fluorescence detection was deployed to detect in-situ the amide bonds of proteins in liquids and at solid liquid interfaces.

195 Characterization of surface contaminants of medical devices

Pollakowski B, Hornemann A, Tyler B, Steven R, Emmer P, Beckhoff B

Advance biomaterials for medical devices need metrology tools for a traceable and reliable analysis to detect and identify defect structures and contaminants. Bis-steramide is a contamination originating from production and packing. Combined grazing incidence X-ray fluorescence analysis and FTIR spectroscopy allow for a traceable analysis of thickness and chemical species of the contaminants.

196 Actinic characterization of EUV Photomasks by EUV Scatterometry

Scholze F, Soltwisch V, Ullrich A, Philipsen V and Burger S

Present Metrology solutions for semiconductor technology are insufficient beyond the 22nm-node. PTB has been working on the development of scattering methods for mask metrology for several years. EUV scattering methods show an excellent performance for the characterization of line structures on EUV photomasks. We commissioned a new Scatterometer capable of measuring 6” size mask substrates.

197 A von Hamos X-ray spectrometer concept based on two cylinder-segment HAPG mosaic crystals

Holfelder I, Müller M, Schlesiger C, Wansleben M, Beckhoff B

A von Hamos spectrometer based on two cylinder-segment mosaic crystals was characterized and compared to a one-crystal spectrometer. A modified pyrolytic graphite, the Highly Annealed Pyrolytic Graphite (HAPG), was used as a dispersive element, which shows a high spectral resolution compared to other mosaic crystals. The results show an increase in resolution when using a double-crystal concept.

198 A diffraction effect inside X-ray area detectors

Gollwitzer C, Krumrey M

When scattering images are recorded using an X-ray area detector with a single-crystalline sensor layer, diffraction in the sensor layer can expose a pattern of lines which overlays the images. We compare images recorded at the FCM beamline of PTB in the tender X-ray range using a PILATUS 1M detector with a theoretical simulation. The effect can be exploited for high-accuracy energy calibration.

CR 114h BESSY VSR - A Variable Pulse Length Storage Ring -

Goslawski P, Ruprecht M, Ries M, Wüstefeld G on behalf of the BESSY VSR project team

This poster will present the upgrade project BESSY VSR for BESSY II

CR 114i Coherent x-ray scattering and imaging with the CXS end station at UE49-SGM

Mishra D, Fohler M, Geilhufe J, Hennecke M, Zieglarski M, Güthling C, Pfau B, Günther C, Noll T, Bischoff P, Engel D and Eisebitt S

Coherent soft X-rays have added a new dimension to imaging techniques at the nanometer length scale. A new end station for coherent X-ray scattering (CXS) has been in operation for a year to address the demand for coherent scattering as well as holographic and ptychographic imaging. We highlight few examples from last year user operations and propose future upgradations envisioned for users.

CR 114j X-PEEM investigation of chemical and electronic surface properties of solution processed perovskite-based thin-film solar cell structures

Hartmann C, Sadoughi G, Wilks RG, Klemm HW, Peschel G, Madej E, Fuhrich AB, Handick E, Raoux S, Schmidt Th, Snaith H, Bär M

X-PEEM investigation of the surface of 300 nm thick $CH_3NH_3PbI_{3-x}Cl_x$ layers on compact TiO_2 shows an inhomogeneous morphology with an incomplete coverage of the substrate. Depending on the degree of coverage, we find indications for an enhanced I-oxidation close to or the formation of metallic Pb in the proximity of (but not right at) the TiO_2 substrate.

Abstracts of Poster Session - Neutron Day

Friday, 11th of December

1 Characterization of Residual Stress State on Inert Gas Welded Joints by Neutron Diffraction at E3 – BER II

Lyamkin V, Cabeza S, Bruno G, Stegemann R.

The material under study was a commercial S235JR sheet with 5mm thickness. Tungsten inert gas (TIG) weld was performed in the middle of two plates. Residual stresses were characterized by neutron diffraction mapping along longitudinal and transversal directions to the weld, and along thickness on top of the plate (weld) and bottom (only heat affected zone).

2 Magnetic properties of the nanocrystalline $DyMnO_3$

Baran S, Dyakonov V, Hoser A, Penc B, Zarzycki A, Szytula A

We report on the X-ray and neutron diffraction and magnetic measurements of the nano-samples of $DyMnO_3$ annealed at temperatures of 800, 850 and 900 C. All the samples are antiferromagnets at low temperatures. The Mn magnetic moments order near 40K while those of Dy below 8.5K. The broadening of magnetic peaks connected with the Dy sublattice suggests a cluster-like character of magnetic ordering.

3 Phase content and neutron diffraction analysis of off-stoichiometric Cu_2ZnSnS_4 (CZTS)

Neldner, Gurieva, Többens, Franz, Whitfield, Schorr

Cu_2ZnSnS_4 (CZTSS) has been proven to be a promising absorber material. Studies on deviation from stoichiometry, distribution of the cations are of great importance to understand solar cell performance. Neutron diffraction was applied to obtain the site occupation of the Cu, Zn and Sn sites in the kesterite structure. The cation site occupation is in agreement with the postulated type defects.

4 Magnetic interactions in $La_{0.7}Sr_{0.3}Mn_{1-x}Me_xO_3$ (Me=Ga, Fe,Cr) manganites

Sikolenko V, Többens D, Karpinsky D, Troyanchuk I, Bushinsky M, Tereshko N, Dobryansky V, Efimova E, and Efimov V

Magnetic properties and crystal structure of $La_{0.7}Sr_{0.3}Mn_{1-x}Me_xO_3$ (Me=Ga, Fe,Cr; x<0.3) have been studied by neutron powder diffraction and magnetization measurements. It is shown that substitution of manganese ions by chromium or gallium ions(x=0.3) leads to phase separation into antiferromagnetic and ferromagnetic phases whereas replacement by Fe ions stabilizes spin glass state(x=0.3)

5 Structural Trends in off-stoichiometric $Cu_2ZnGeSe_4$ compound semiconductors

Gunder, Schorr

Substituting Sn by Ge in kesterite-type solar energy absorbers $Cu_2ZnSn(S,Se)_4$ (CZTSSe) facilitates the possibility to tune the bandgap energy. A series of CZGSe powder samples was synthesized and analyzed by neutron diffraction. In conjunction with quantitative WDX spectroscopy the neutron diffraction data is used to deduce both the cation distribution as well as the point defect concentration.

6 Structure-property relations in chalcopyrite based intermediate band solar absorber materials

Marquardt, Stephan, Schorr

By adding transition metals into a well-known semiconductor absorber, we try to create an intermediate band. With this absorbers efficiencies of 63% are proposed. We focus our study on the solubility of MnS/Cr_2S_3 into $CuGaS_2$, the cation distribution and the understanding of resulting defects. The powder samples have been synthesized by solid state reaction and investigated by neutron diffraction.

7 Intrinsic point defects formation in off-stoichiometric $Cu_2ZnSnSe_4$

Valle-Rios LE, Gurieva G, Whitfield P, Franz A, Többens D, Schorr S

Neutron scattering length of Cu and Zn is different, therefore is possible to distinguish between their site occupation in the crystal structure. Rietveld refinements of E9 collected data followed by the average neutron scattering length analysis method lead the determination of cation distribution and the formation of intrinsic point defects, which differ according different off-stoichiometry

8 Structural characterization of Re-substituted lanthanum tungstates $La_{5.4}W_{(1-x)}Re_{(x)}O_{12-delta}$ (x=0, 0.2) by neutron diffraction

Fantin A, Scherb T, Seeger J, Schumacher G, Meulenberg WA, Dittmeyer R, Banhart J

The structural characterization of the proton conductor $La_{5.4}W_{1-x}Re_xO_{12-d}$ (0<=x<=0.2) is presented. The series boundaries (x=0,0.2) in dry/D_2O conditions will be compared through neutron diffraction (1.5K<=T<=1200K) due to the insufficient contrast between W (Z=74,b=4.86fm) and Re (Z=75,b=9.2fm) against X-Rays. Thermogravimetry, composition studies and remaining static disorder are also addressed.

9 The crystal structure of $MaPbI_3$: a complementary neutron and synchrotron X-ray diffraction study

Franz A, Toebbens DM, Schorr S

In recent years the interest became focused on organic-inorganic perovskites as a future solar energy material. Our focus lays in CH_3 NH_3PbI_3 on which neutron diffraction (BER II, E9) and synchrotron X-ray diffraction experiments (BESSY II, KMC-2) beamline were performed. The results of this structural study with emphasis on statistic disorder of the methylammonium molecule will be discussed.

10 Combination of 3D-cross correlated light scattering with small-angle neutron scattering

Günther A, Hertle Y, Clemens D, Bookhold J, Chu F, Ballauff M, Hellweg T

The combination of 3D-cross correlation light scattering with the small-angle neutron scattering instrument V16 at the Helmholtz-Zentrum in Berlin will enable researchers, particularly in the field of soft condensed matter, to perform simultaneously neutron and light scattering experiments on highly concentrated samples under exact the same conditions for both scattering experiments.

11 Impact of Polyallylamine-hydrochlorid (PAH) on DMPC-Oligobilayers investigated with Combined In Situ Neutron Reflectivity and ATR-FTIR Measurements

Schwörer F, Trapp M, Steitz R, Dahint R,

The time-of-flight reflectometer BioRef was employed to characterize the structure and molecular conformation of thin lipid films by adding PAH. For DMPC lipid coatings we observed enhanced mechanical stability and a swelling behavior which is strongly dependent on the concentration of the polyelectrolyte solutions. The experiments provide first insight in mechanisms of wear reduction in joints.

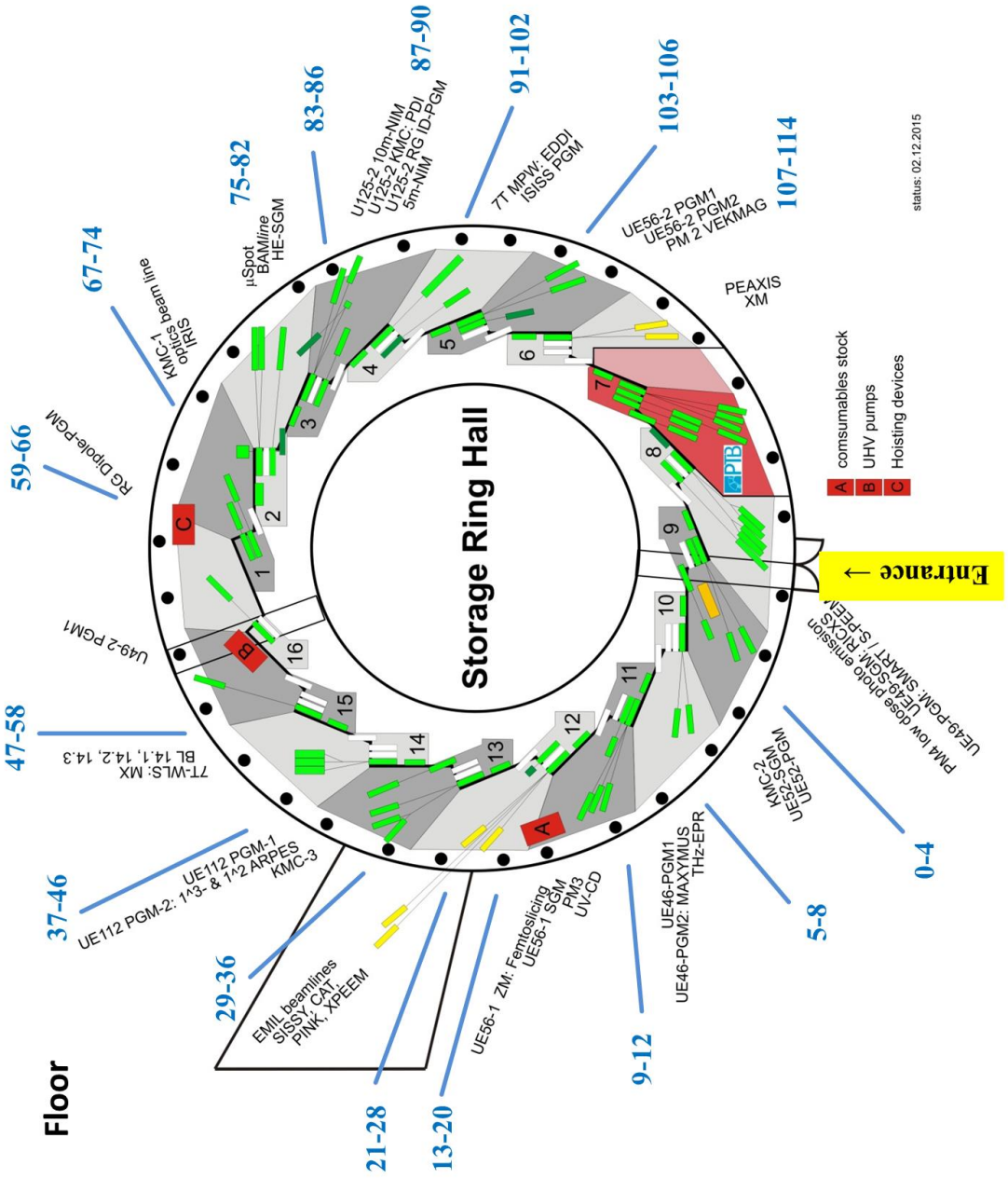
12 Neutron Resonance Spin-Echo upgrade at the three-axis spectrometer FLEXX

Groitl F, Keller T, Quintero-Castro DL, Habicht K

The NRSE option of the cold triple axis spectrometer FLEXX at the BER II neutron source at HZB, Berlin, has been rebuilt as part of a major upgrade program. Redesigned NRSE bootstrap coils allow for an efficient use of the larger beam cross section. Larger coil tilt angles enable measurements on steeper dispersions. The new design of the spectrometer arms results in a more compact instrument and increases the accessible Q-range in Larmor diffraction geometry.

Floorplan of Poster Session – Science Day at BESSY II

Thursday, 10th of December



Floorplan of Poster Session – Science Day at BESSY II

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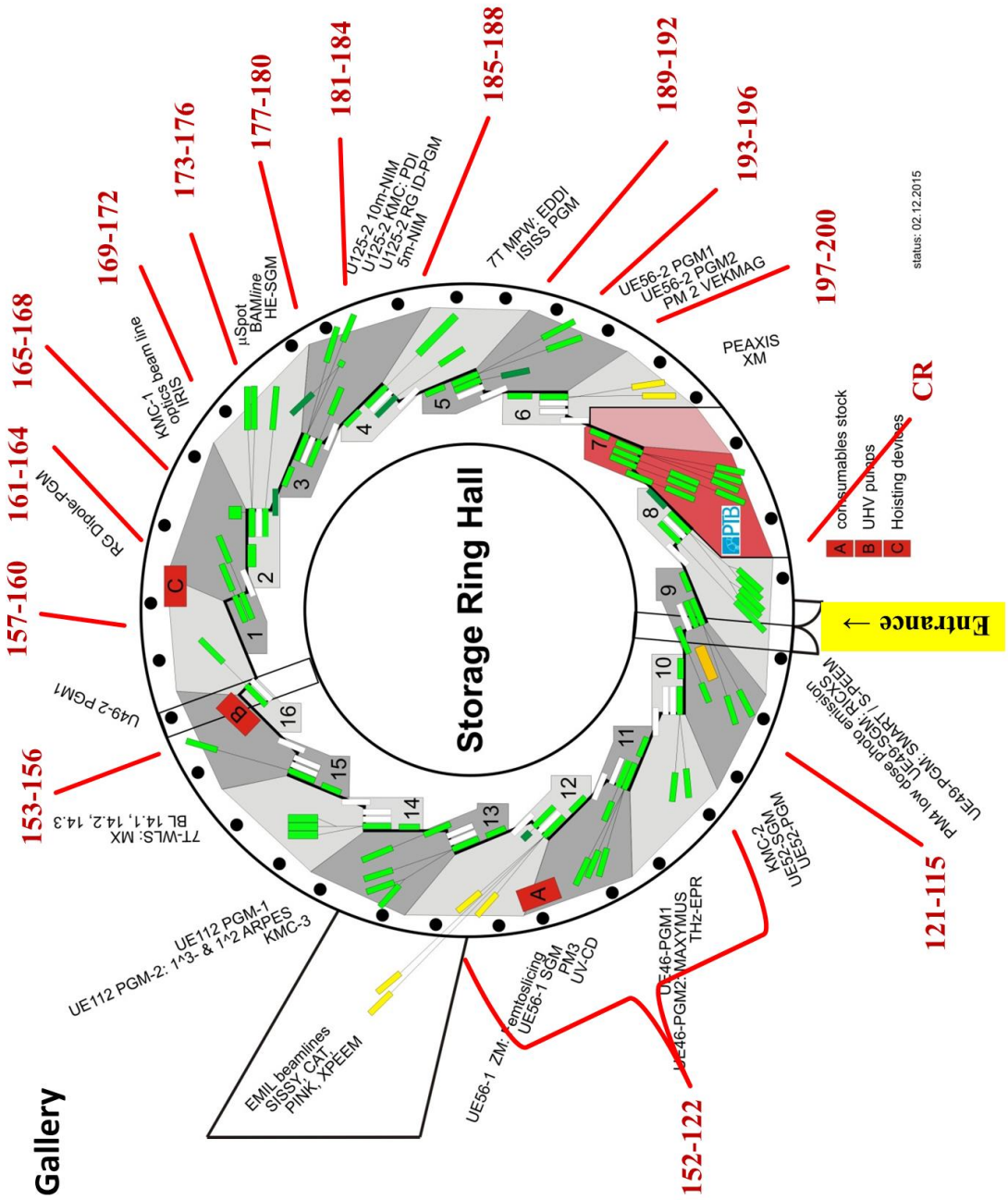

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Procedures for electing members of the HZB User Committee

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 2015 is
27. November 2015 [00:01] – **11. December 2015** [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

Francesco Allegretti	Technische Universität München, Deutschland	Physicist Methods: PES, XPD, NEXAFS, XSW, Resonant Auger-Raman Spectroscopy, STM, TPD Area of interest: organic and oxide thin films, surface-supported low-dimensional nanostructures, determination of adsorbate and surface structure **Photons**
Carolin Schmitz-Antoniak	Forschungszentrum Jülich GmbH, Deutschland	Physicist Methods: XANES, XMCD, EXAFS Area of interest: magnetism of nanoscale systems (anoparticles, clusters, thin films) **Photons**

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:

Carolin 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
Freundeskreis Helmholtz-Zentrum Berlin e.V.
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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:	

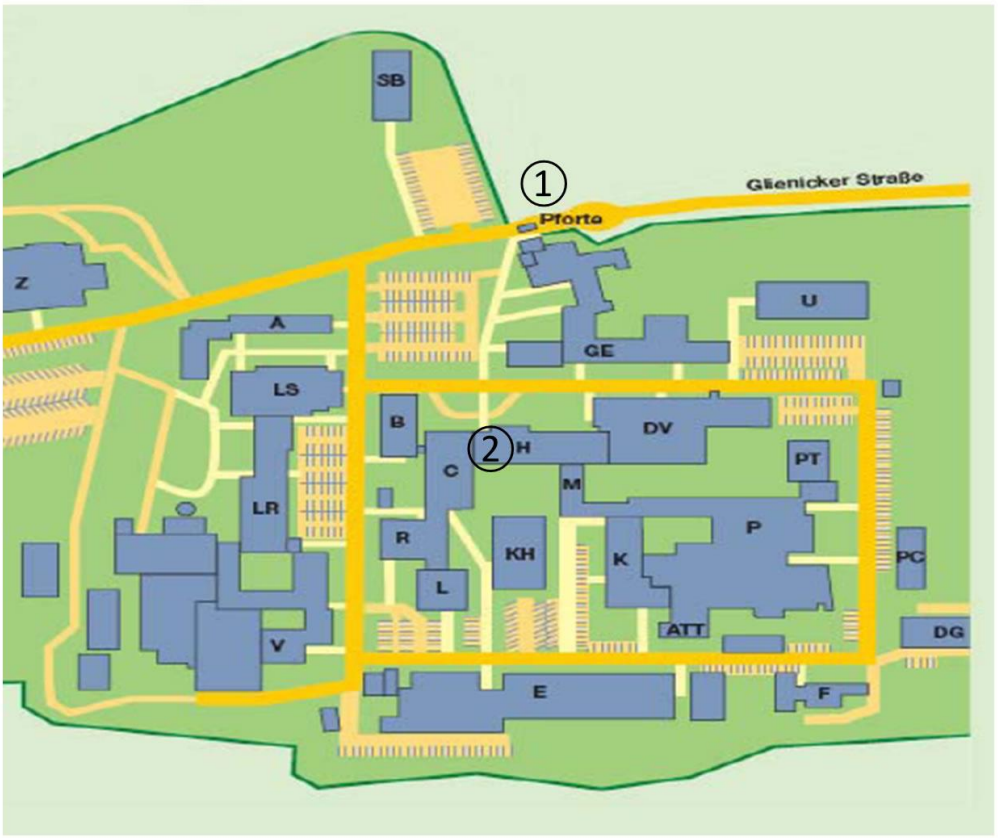
Die jährlichen Mitgliedsbeiträge betragen zur Zeit für natürliche Personen EUR 40,-, für juristische Personen EUR 150,-, EUR 100,- oder EUR 50,-, für Studenten EUR 10,-. / The regular annual membership fees amount to EUR 40,- for natural persons, EUR 150,–/100,-/50,- for legal entities, EUR 10,- for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

Helmholtz-Zentrum Berlin
Lise-Meitner Campus
Wannsee



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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 2016

Call for Proposals 2016/II

HZB kindly invites you to submit proposals for the next allocation period from August 2016 to February 2017 for BESSY II and BER II.

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

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

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

http://www.helmholtz-berlin.de/user/beamtime/guide_en.html

www.helmholtz-berlin.de/user/beamtime/proposals/index_en.html