HZB Helmholtz Zentrum Berlin

10TH JOINT BER II AND BESSY II USER MEETING

Dec. 5-7, 2018

Celebration of 20 Years of Beam and Light at BESSY II, December 5th

Keynote Lecture:
Gisela Schütz (MPU IS Stuttgart)

Public Lecture:
Caterina Biscari (ALBA)

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

Invited Talks:
Benedetta Casu (University Tübingen)
Kristina Edstrøm (University of Uppsala)
Manuel Bibes (CNRS)
Alan Williams (The Wallace Collection Conservation, London)
Nønne Prisle (University Oulu)
Norbert Koch (HUB)
Holger Dau (FU Berlin)
Emile Rienks (HZB, TU Dresden)
Jessica Huss (MPI of Colloids and Interfaces Golm)
Sonja Lorenz (University of Würzburg)

Satellite Workshop:
15 years of MX at BESSY II. The workshop will take place on Friday, December 7th at the Wilhelm-Conrad-Röntgen-Campus in Adlershof.

Wilhelm-Conrad-Röntgen Campus (Berlin-Adlershof), WISTA and Lise-Meitner-Campus (Berlin-Wannsee)

http://hz-b.de/um2018

Helmholtz-Zentrum Berlin

für Materialien und Energie GmbH

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Dear users and friends,

Welcome to the 10th Joint BESSY II and BER II User Meeting of HZB, which brings together users from the neutron and the synchrotron radiation source at our sites in Berlin Wannsee and Adlershof.

This year's User Meeting is a special one, we celebrate 20 years of beam, light and experiments at BESSY II and we look back to a very successful evaluation of the HZB's large-scale facilities by an international review panel which confirmed the highest quality of the science performed at BESSY II. One of the milestones in 2018 was the installation of the tender X-ray undulator CPMU17 which will complement the soft X-ray undulator UE48 to provide radiation from 60 eV to 6 keV at our CAT and SISSY experiments in the EMIL@BESSY II laboratory.

In the same shutdown, the PSF wavelength shifter feeding the MX beamlines was successfully refurbished and the Landau Cavities were brought back, enabling again higher ring currents of up to 300 mA. Unfortunately, the overhaul of the BAM multipole wiggler resulted in a cold leak, which forced us to remove the insertion device temporarily from the ring.

Always looking for improvement, the synchrotron radiation source BESSY II has extended its portfolio of state-of-the-art beamlines with PEAXIS and an upgrade for circular polarization at the RGBL Dipole, both in full user operations now. The RGBL insertion device beamline is awaiting friendly users, while ENERGIZE, the new U49/2-PGM-2, BEIChem and METRIXS are on their way.

Tailored filling pattern of the storage ring and specific bunch characteristics were further developed and implemented to increase the flexibility of our storage ring even further. The "two orbit operation" with distinct filling patterns stored simultaneously on two independent orbits has been tested successfully in a dedicated user week in February.

CALIPSOplus, a European integrated activity for advanced communities funded within Horizon2020 goes remarkably well: the dissemination and twinning project with the aim of lowering barriers for using world-class accelerator-based light sources in Europe and the Middle East, and to promote and support international exchange and transnational access, is highly recognized. Seminars and lectures have been given in 15 universities in 6 countries. As a result, 7 twinning teams have been established who submitted already their first proposals.

The comprehensive quality management system for User Service at BESSY II, implemented in 2017, has been review-audited by TÜV Süd and received highest appreciation. The quality management system has received a lot of interest from other facilities.

At BER II we face the last year of operation with 10 competitive instruments at highest possible standards, among them the HFM/EXED instrument, which enables experiments in the strongest continuous magnetic field for neutron scattering worldwide. Some instruments were already transferred to other neutron sources, like for example the reflectometer BioRef. It is

now fully operational and in user service under the name “Spatz” at the OPAL neutron source, which is part of the Australian Nuclear Science and Technology Organisation (ANSTO) in Sydney.

Complementing the large-scale facilities, HZB provides state-of-the-art laboratories as well as unique equipment for the scientific community. At both sites, a competitive X-ray CoreLab offers a multitude of experimental techniques, ranging from diffraction, reflectivity, to stress and strain analysis. EMIL@BESSY II - which was highlighted in the review as a significant new opportunity for interdisciplinary research and an important new direction for the future - the microscopy CoreLab (participating in the ZEISS labs@location program), HySPRINT (for Hybrid Silicon Perovskite Research), the Competence Centre Thin-Film and Nanotechnology for Photovoltaics Berlin PVcomB and the CoreLab Quantum Materials round off the suite of infrastructures available to all users.

A highlight of this year’s Joint User Meeting is the public lecture given by Caterina Biscari, the director of the synchrotron source ALBA and vice chair of LEAPS. The League of the European Accelerator based Photon Sources is a consortium of 16 facilities pushing forward European cooperation, development and scientific progress.

The Innovation Award and the Ernst-Eckhard-Koch Prize bestowed by the “Freundeskreis Helmholtz-Zentrum Berlin e.V.” once again bear witness to the outstanding research performed by our users and colleagues.

The social highlights of this year’s user meeting are certainly the 20 years of photon science at BESSY II celebration taking place at the end of the Synchrotron Day and, once again, the Berliner Buffet, which is kindly sponsored by the companies taking part in the industrial exhibition. Moreover, intense scientific discussions can be expected to take place during the two poster session, which received more than 180 poster registration! The divers programme reflecting the remarkable range of research performed at HZB includes also two young scientists sessions to highlight the contributions of this group.

A satellite workshop “15 Years MX@BESSY” completes the meeting.

We thank you all for joining the User Meeting and look very much forward to inspiring and fruitful discussions, to the exchange of exciting new ideas and future collaborations beyond it.

A cordial welcome to you from all of us. Enjoy the meeting and let’s celebrate together.

Sincerely,

Prof. Dr. Bernd Rech
Designated Scientific Director

Prof. Dr. Jan Lüning
Designated Scientific Director

Contents

Wednesday, December 5th, 2018:
Young Scientists and Synchrotron Day

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

13:30 – 19:00	**Registration and Vendor Exhibition**	WISTA Centre
14:00 – 15:40	**Synchrotron Session** *(Chair: Christian Jung)*	Bunsen Auditorium
14:00	*Bernd Rech (HZB)* **Welcome**	
14:10	*Jan Lüning (HZB)* **BESSY II: Photon Science**	
14:40	*Andreas Jankowiak (HZB)* **Accelerator Operation and Projects @ HZB**	
15:00	*Robert Seidel (HZB)* **Sol³PES**	
15:20	*Axel Knop-Gericke (FHI)* **Ambient pressure x-ray photoelectron spectroscopy of catalytically active solid-gas phase and solid-liquid interfaces: Status and new options at EMIL**	
15:40 – 16:00	**General Discussion**	Bunsen Auditorium
16:00 – 16:30	**Coffee Break**	WISTA Centre
16:30 – 18:00	**Young Scientists Session** *(Chair: Carolin Schmitz-Antoniak)*	Bunsen Auditorium
16:30	*Samuel Edwards (Trinity College Dublin)* **An X-ray spectroscopic investigation of uranium minerals relevant to the storage of spent nuclear fuels**	
16:45	*Vesna Zivanovic (HU Berlin)* **Gold nanoparticles and drugs in cells: Insights from cryo-XRT and vibrational spectroscopy**	
17:00	*Saša Petrović (MDC Berlin)* **Structural basis of ASPL-mediated regulation of p97 methylation by METTL21D**	
17:15	*Jian Ren (HZB)* **An ex-situ study of the structure-property relationship in highly efficient carbon nitride photocatalysts for hydrogen evolution**	
17:30	*Fabian Düll (University of Erlangen)* **Bimetallic Nanocluster Arrays as Model System for Catalysis**	
17:45	*Aisha Aqeel (University of Nürnberg)* **Bragg Scattering Ferromagnetic Resonance on a chiral magnetic insulator**	
	Sparkling wine reception in the vendor exhibition area	
19:00 - 21:30	**Celebration 20 Years of Beam and Light at BESSY II** **Live music, sketches, "Currywurst" and more**	Bunsen Auditorium

Thursday, December 6th, 2018:
Science Day

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

9:00 – 16:00	**Vendor Exhibition**	WISTA Centre
8:30 – 17:30	**Registration**	WISTA Centre
11:30 – 17:30	**Poster Set-up**	BESSY II
9:30 – 9:40	**Opening** *Bernd Rech/Jan Lüning (HZB)*	Bunsen Auditorium
9:40 – 10:10	**Keynote Lecture** *(Chair: Simone Raoux)* *Gisela Schütz (MPU IS Stuttgart)* **Time-resolved microscopy with soft x-rays**	
10:10 – 10:40	**Coffee Break and Vendor Exhibition**	WISTA Centre
10:40 – 12:20	**Oral Presentations I** *(Chair: Catherine Dubourdieu)*	Bunsen Auditorium
10:40	*Maria Benedetta Casu (University of Tübingen)* **Nanoscale studies of organic radicals: Surface, interface, and spinterface**	
11:00	*Kristina Edstrøm (University of Uppsala)* **Title to be announced: Battery Research**	
11:20	*Manuel Bibes (CNRS)* **Mapping and harnessing mesoscopic charge and spin textures in quantum oxide materials**	
11:40	*Alan Williams (The Wallace Collection Conservation, London)* **Neutron techniques in cultural heritage**	
12:00	*Nønne Prisle (University of Oulu)* **How the behavior of molecules in cloud droplets affect global climate**	
12:20 – 13:30	**Lunch Break**	(Canteens on site)
13:30 – 15:10	**Oral Presentations II** *(Chair: Svante Svensson)*	Bunsen Auditorium
13:30	*Norbert Koch (HU Berlin)* **Electronic properties of 2D semiconductors: from single crystals to 2D powders**	
13:50	*Holger Dau (FU Berlin)* **Nickel-iron catalysts for electrochemical water oxidation – redox synergism investigated by in-situ X-ray spectroscopy with millisecond time resolution**	

14:10	*Emile D. L. Rienks (HZB, TU Dresden)* **Samarium hexaboride is a trivial surface conductor**	
14:30	*Jessica C. Huss (MPI of Colloids and Interfaces Golm)* **Climate-dependent heat-triggered opening mechanism of Banksia seed pods**	
14:50	*Sonja Lorenz (University of Würzburg)* **Regulatory mechanisms in HECT ligases**	
15:10 – 15:40	**Coffee Break and Vendor Exhibition**	WISTA Centre
15:40 – 15:50	*Christian Papp (University of Erlangen-Nürnberg)* **Report from the user committee**	Bunsen Auditorium
15:50 – 17:00	**Bestowal of Prizes: Friends of Helmholtz-Zentrum Berlin e.V.** *(Chair: Mathias Richter)*	Bunsen Auditorium
17:00 – 18:00	**Public Lecture** *(Chair: Benedetta Casu)* *Caterina Biscari (ALBA)* **LEAPS, coordinating and integrating European capacities**	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 7th, 2018:
Young Scientists and Neutron Day

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

9:00 – 9:30	**Registration**	(LMC-Foyer)
9:30 – 10:30	**Neutron Session** *(Chair: Klaus Habicht)*	(Lecture Hall LMC)
9:30	*Bernd Rech/Jan Lüning (HZB)* **Opening**	
9:40	*Fabiano Yokaichiya (HZB)* **Unveiling the Drug Delivery Systems using Small Angle Neutron Scattering (SANS)**	
10:00	*Stavros Samothrakitis (ASCR)* **Three-dimensional Laue neutron diffraction for grain mapping and reconstruction of polycrystalline materials**	
10:20	*Veronika Grzimek (HZB)* **Molecular mechanism of hydrogen sorption in CAU metal-organic frameworks**	
10:30 – 11:00	**Coffee Break**	(Café Jahn)
11:00 – 12:30	**Young Scientists Session** *(Chair: Michael Tovar)*	(Lecture Hall LMC)
11:00	*Stanislav E. Nikitin (MPI Dresden)* **Decoupled spin dynamics in the rare-earth orthoferrite $YbFeO_3$: Evolution of magnetic excitations through the spin-reorientation transition**	
11:15	*Christian Pflug (Uni Leipzig)* **Crystal Structure refinement of luminescent materials $NaMgH_{3-x}F_x$ by powder neutron diffraction**	
11:30	*Annekatrin Sill (Uni Greifswald)* **Entanglement in polyelectrolyte multilayers**	
11:45	*Tobias Thiede (BAM)* **An Assessment of Surface and Bulk Residual Stress in Selective Laser Melted Inconel 718**	
12:00	*Camilla Evangelisti (ZSW Ulm)* **In-situ analysis using neutron radiography of porous nickel materials for alkaline water electrolysis**	
12:15	*Torben Pfaff (JLU Giessen)* **Comparative Microstructural Analysis of Non-Graphitic Carbons (NGCs) based on Wide-Angle X-Ray (WAXS) and Neutron (WANS) Scattering**	
12:30 – 14:00	**Poster Session and Lunch**	(Café Jahn)

Abstracts of the Young Scientists Session - Synchrotron Day

Wednesday, 5th of December

S. Edwards 05.12.18, 16:30

An X-ray spectroscopic investigation of uranium minerals relevant to the storage of spent nuclear fuels

S.J. Edwards[1], E. Weschke[2], R.J. Baker[1]

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2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

The safe storage and management of spent nuclear fuels (SNF) is an international problem with many serious repercussions if done improperly. The ongoing challenge of proper storage of SNF requires an understanding of speciation of the actinides to minimize environmental contamination. The hexavalent uranyl ion (UO_2^{2+}) is water soluble, but with some environmentally relevant ions it can form insoluble precipitates such as uranyl phosphates and silicates[1]. Previous studies have shown transuranic (e.g. Np) incorporation into uranyl phosphates hinders environmental contamination[2], but the stability over long periods of time are unknown.
An area of high interest within actinide chemistry is that of cation-cation interactions (CCI). Co ordination between an oxo atom of an actinyl, i.e. uranyl, and a metal actinide centre can lead to a multitude of structural formations[3]. CCI's within uranyl compounds (VI) show peculiar behaviours including possible deviations in the magnetic ordering via large exchange pathways[4].
Using a high field diffractometer (UE46_PGM-1, BESSY II), the oxygen K-edge, uranium $N_{4/5}$ and copper L-edge were measured for cuprosklodowskite $[Cu(UO_2)_2(SiO_3OH)_2].6H_2O$ and metatorbernite $[Cu(UO_2)_2(PO_4)_2].8H_2O$ as a spectroscopic method to investigate CCIs and the electronic structure of these species.

References:
[1] Inorganic Chemistry 52, 3510 (2013)
[2] Crystal Growth & Design 13, 386 (2013)
[3] Journal of the American Chemical Society 126, 2676 (2004)
[4] Journal of Solid State Chemistry 213, 1 (2014)

Gold nanoparticles and drugs in cells: Insights from cryo-XRT and vibrational spectroscopy

V. Živanović[1], D. Drescher[1], P. Schrade[2], G. P. Szekeres[1], S. Werner[3], P. Guttmann[3], S. Bachmann[2], G. Schneider[3], C. Arenz[1], J. Kneipp[1]

1 Humboldt-Universität zu Berlin, Germany
2 Charité Universitätsmedizin, Germany
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

In cells, tricyclic antidepressants (TCA) enrich in lysosomes and influence the lipid content of their membrane.[1] Gold nanoparticles, which can serve both as optical probes as well as transporters for TCA,[2] accumulate in the lysosomes and can interact with the lysosomal membrane.[3] To understand the interaction of TCA with lysosomes and gold nanoparticles, surface-enhanced Raman scattering (SERS) and cryo X-ray tomography (cryo-XRT) are combined. Cryo-XRT provides details on the morphology of the gold nanoparticle accumulations in the presence of TCA. These data are correlated with SERS, which can give information on the lipid composition of lysosomes.[4] The spectra indicate a substantial influence of TCA on lysosome biochemistry. The results of this work can be used to better understand the mechanisms of action of TCA.

References:
[1] Arenz Cell. Physiol. Biochem. 26, 1, (2010)
[2] J. Phys. Chem. C 121, 41, (2017)
[3] Nanoscale 5, 19, (2013)
[4] J. Phys. Chem. Lett. 9, (2018)

Structural basis of ASPL-mediated regulation of p97 methylation by METTL21D

S. Petrović [1,2], U. Heinemann [1,2]

1 Max Delbrück Center for Molecular Medicine, Germany
2 Freie Universität Berlin, Germany

The hexameric ATPase p97/VCP (valosin containing protein) is a chaperone that belongs to the family of AAA+ proteins (ATPases associated with diverse cellular activities). It is involved in a broad range of cellular processes, such as DNA repair, cell cycle regulation, ubiquitin-mediated protein degradation, and other [1]. The function of p97 is regulated by a number of adaptor proteins and post-translational modifications [2]. The adaptor protein ASPL (alveolar soft-part sarcoma locus) has been investigated in our group biochemically and structurally, showing that ASPL regulates p97 activity by remodeling it from a hexamer into a heterotetrameric complex containing two monomers of p97 and two molecules of ASPL [3]. METTL21D, also known as VCP-KMT (VCP-lysine methyltransferase), trimethylates p97 specifically at Lys315 [4,5]. Trimethylated Lys315 is ubiquitously present in the intact hexameric form of endogenous p97 inside the pore, but it is inaccessible to METTL21D. ASPL promotes methylation by disassembling the hexameric form of p97, thereby making Lys315 accessible to METTL21D. Here we present the first crystal structure of a methyltransferase from the METLL family, METTL21D, bound to its target chaperone p97 in presence of its remodeling adaptor protein ASPL, adenosine-diphosphate (ADP) and the cofactor S-adenosyl-L-methionine (SAM). The structure shows the importance of p97 remodeling by ASPL and potentially other remodeling adaptor proteins to enable modification of inaccessible residues and to create new interaction interfaces.

[1] Biochem. J. 474, 2953 (2017)
[2] Front. Mol. Biosci. 4, 1 (2017)
[3] Nat. Commun. 7, 13047 (2016)
[4] Nat. Commun. 3, 1038 (2012)
[5] PLoS Genet. 9, e1003210 (2013)

An *ex-situ* study of the structure-property relationship in highly efficient carbon nitride photocatalysts for hydrogen evolution

J. Ren[1,2], N. Meng[3], B. Zhang[3], T. Petit[1]

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2 Freie Universität Berlin, Germany
3 Tianjin University, China

Since 2009, polymeric carbon nitride (PCN) photocatalysts have attracted substantial attention due to their abundant cheap precursors, chemical stability and modification flexibility.[1] However, the photocatalytic performances of pristine PCN are relatively low because of its poor dispersion in water, low electric conductivity and rapid rate of charge-carrier recombination. Optical, electronic, mechanical and chemical properties of PCN materials can be manipulated by changing the size, composition, dimension and shape of their reactive nanodomains. Recently, the oxygen-containing and primary amino groups decorated atomically-thin PCN nanosheets were prepare via a facile continuous thermal treatment strategy in air/NH_3 atmospheres to dramatically enhance the photocatalytic hydrogen generation performance.[2]

In this presentation, the structure-property relationship in highly efficient carbon nitride photocatalytsts, as determined from various spectroscopy methods will be discussed. Especially, ultraviolet and X-ray photoemission spectroscopies (PES), Fourier transformed infrared (FTIR) spectroscopy and synchrotron-based X-ray absorption spectroscopy (XAS), performed at the BESSY II photon source, were applied to characterize in more details PCN materials before and after modifications. These measurements reveal that the tailored modifications on the structure and chemistry endow the PCN nanosheets with hydrophilic surfaces, more negative conduction-band edge and strong Lewis basicity, thus synergistically leading to highly efficient H_2 evolution.

This research could open new perspectives to design PCN with enhanced photocatalytic performance. It also demonstrates that combined infrared, UV and X-ray-based characterization methods provide complementary information about structure and properties of carbon nanomaterials.

References:
[1] Nat. Rev. Mater. 2, 17030 (2017)
[2] Energy Environ. Sci. 11, 566 (2018)

F. Düll 05.12.18, 17:30

Bimetallic Nanocluster Arrays as Model System for Catalysis

Fabian Düll[1], Udo Bauer[1], Florian Späth[1], Philipp Bachmann[1], Johann Steinhauer[1], Hans-Peter Steinrück[1], Christian Papp[1]

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Nanoclusters are an intriguing model system for catalysis, as they bridge the materials gap between single crystals and real catalysts by introducing various, different facet and edge sites. We utilize the Moiré pattern of graphene on Rh(111) as a template for growth of the nanoparticles. Thereby, well-ordered arrays of separated nanoclusters with a narrow size distribution are formed. As no molecules adsorb to the chemically inert graphene substrate, spillover and reverse-spillover processes are avoided. Such nanoclusters arrays were studied in detail by our group in the past using *in situ* high-resolution X-ray photoelectron spectroscopy [1, 2]. Now, we use this in-depth knowledge to handle more complex processes and systems, *e.g.,* bimetallic alloy nanoclusters [3].

Alloy catalysts have, in many cases, superior properties compared to their single metal counterparts. Alloying Pt with Pd is used, *e.g.*, to enhance the performance and stability of Pt catalysts in reactions that include an oxygen reduction, or to stabilize species like aldehydes that would decompose on the single metals.

By utilizing our molecular beam / XPS setup and a tunable high-flux undulator X-ray source (UE56/2-PGM2), we investigated the site occupation and dynamic changes of the metal distribution during adsorption and thermal treatment of CO layers on PdPt alloy nanocluster arrays on graphene/Rh(111). Annealing of the as-prepared nanoclusters to 550 K after exposure to CO leads to a restructuring of the nanoparticles towards a more 3D shape. At the same time, the Pt atoms at the cluster edges are replaced by Pd atoms, while the facets are dominated by Pt. This procedure leads not only to a restructuring but also to a stabilization of the nanoclusters, as repeated CO adsorption and desorption cycles cause no further changes. Interestingly, we, however, observe dynamic changes during TPXPS or when applying a CO- or O_2-stream using a supersonic molecular beam at constant temperatures. Up to 340 K, CO molecules rearrange from terrace to edge sites. Starting above 360 K, Pt edges are formed again. Yet, they only exist at elevated temperatures in the presence of CO, and disappear when the system cools down in a vacuum.

References:
[1] J. Phys. Chem. C 118, 25097 (2014)
[2] ACS Catal. 5, 2397 (2015)
[3] Phys. Chem. Chem. Phys. 20, 21294 (2018)

Bragg Scattering Ferromagnetic Resonance on a chiral magnetic insulator

S. Pöllath[1], A. Aqeel[2], A. Bauer[2], C. Luo[2,3], H. Ryll[3], F. Radu[3], C. Pfleiderer[2], C.H. Back[1,2]

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2 Technische Universität München, Germany
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Ferromagnetic resonance is a long-time established method to measure magnetic parameters of collinear ferromagnets and recently in some new types of chiral magnets with spin modulation lengths in the order of 100nm [1]. In this work, we show a novel way to explore ferromagnetic resonance (FMR) using Resonant elastic X-ray scattering (REXS) [2] of a structural Bragg peak as well as its magnetic satellite peaks – referred as Bragg-FMR. With the Bragg-FMR, we study the collective spin excitations directly in reciprocal space. Here, we measure the ferromagnetic resonance of the helical, field-polarized and skyrmion lattice phase of a chiral magnetic insulator Cu_2OSeO_3. With this novel technique, we phase selectively measure the three theoretically predicted skyrmion eigenmodes with large sensitivity and reveal enhanced helical ordering when the system is excited in resonance.

[1] Phys. Lett. 111, 032408 (2017)
[2] Nano Lett. 16, 3285 (2016)

Abstracts of the Keynote and Public Lecture - Science Day

Thursday, 6th of December

Time-resolved microscopy with soft x-rays

G. Schütz[1] and M. Weigand[1]

1 Max Planck Institute for Intelligent Systems, Germany

Advanced soft x-ray microscopy in the transmission mode (STXM) provide an element-specific visualization of nanostructures, with lateral resolution down to below 15 nm using Fresnel zone plate optics and 5 nm on the basis of coherent imaging via ptychography. In addition, chemical and magnetic maps of the specimen can also be created using the spectroscopic techniques of NEXAFS and XMCD as contrast mechanism. Finally, fast single photon detectors allow stroboscopic imaging with time resolutions according to the flash length of the synchrotron (typically 10 – 100 ps). This gives excellent possibilities to investigate nanoscale data processing units and model devices covering the field of spintronics and magnonics, where the magnetization dynamics appearing in the 0.1 to 10 GHz range play the key role.
At the MAXYMUS endstation of BESSY II time and spatially resolved STXM techniques have been developed providing an unprecedented combination of 15 nm lateral and 10 ps time resolution using multi-bunch and low-alpha light as probe. The samples are electronically pumped by RF or pulse excitation up to frequencies of 30 GHz and 30 ps pulse lengths. As a scanning probe device sophisticated lock-in techniques can be used enabling to create magnetization movies in arbitrary fields of views (from nm to mm) even at low contrasts of 10^{-3}. The current up-grade by adding a laser in collaboration with the Max Born Institute allows thermal / optical pumping and will also provide (sub) ps excitation. The available shorter pulse lengths accommodate excellently the upcoming BESSY VSR, closing the gap to the Free Electron Lasers and opening new and world-wide unique exciting prospects for psec and nm resolved physics, chemistry and material science.

References:
Science 337, 1075 (2012)
Nature 444, 461 (2008)
Nature Nanotechnology 11, 948 (2016)
Nature Materials 15 501 (2016)
Nature Physics 13, 170 (2017)
Nature Electronics 1, 288 (2018)

LEAPS, coordinating and integrating European capacities

C. Biscari[1,2]

1 ALBA Synchrotron, Spain
2 LEAPS Vice Chair

The European Synchrotrons and Free Electron Lasers have a long history of fruitful collaborations in a healthy competitive environment. Now they are joining forces to master the challenges of the next decades by adding their capacities in smart specializations, and developing together the European strategy for photon science.
LEAPS, the League of European Accelerator-based Photon Sources, includes sixteen institutions as founding members, hosting national facilities plus two international ones, namely ESRF and EU XFEL, and representing a total community of 25000 researchers.
Scientific and technical developments for next generation sources, innovation programs, technological transfer for industrial capacitation, better services to users, opening to the world, outreach to society, are the main stream of the collaboration.
LEAPS was launched one year ago in Brussels, with the presence of the European Commission, calling to a new paradigm of co-funding participation of national funding agencies to such kind of programs.
During the last few months, pilot project proposals, aimed at developing specific strategic technologies and new services to the community, have been prepared and then presented during the first LEAPS Plenary Meeting, recently held in Hamburg. This is the first practical result of the collaborative spirit and efficiency of the initiative and useful to develop the models for more ambitious projects in view of participation in Europe.
The Plenary Meeting had another important milestone: SESAME became the first LEAPS Associate. SESAME is hosting its first users and is a great example of the peaceful role of the science voice.

Abstracts of the Oral Presentations - Science Day

Thursday, 6th of December

Nanoscale studies of organic radicals: Surface, interface, and spinterface

M.B. Casu[1]

1 University of Tübingen, Germany

Our technological development was made possible also due to the discovery and synthesis of new materials with characteristics at the nanoscale that are designed for specific purposes. This “on purpose” approach, joined to the development of preparation and growth methods, led to use thin films rather than bulk materials in devices. For several decades thin films, surfaces and interfaces have been intensively investigated. Indeed, device performances rely on the optimized match of thin films of different nature, such as organic/inorganic semiconductors and metals for contacts. Surprisingly, in comparison, little attention has been devoted to the deposition of organic radicals on a substrate. This might be due to the fact these materials are considered not stable enough for evaporation.
In this work, we demonstrate that it is possible to evaporate and deposit organic radicals onto well-defined surfaces under controlled conditions, without degradation. Using soft X-ray spectroscopies, performed also at synchrotrons, we investigate thin film processes, surfaces and interfaces at the nanoscale, when organic radicals are deposited on metal and metal oxide surfaces. We suggest how to design organic radicals bearing in mind the thermodynamic factors that govern thin film stability, with the purpose of obtaining not only a chemically stable radical, but also stable thin films. We investigate the thermal and air stability of the deposited films, and we explore the influence of the surface/radical chemical bond and the role of surface defects on the magnetic moment at the interface. We find that organic radicals are physisorbed and keep their magnetic moment on inert and passivated surfaces, while defective sites such as oxygen vacancies or presence of OH groups lead to chemisorption of the organic radicals on the surface with quenching of their magnetic moment.
Our work shows that the use of X-ray based techniques represents a powerful approach to reveal the mechanisms governing complex interfaces, such as radical/metal and radical/metal-oxide where it is important to describe both charge and spin behavior (spinterfaces). A deep understanding of stable radical/inorganic spinterfaces may open the way to use radicals in solid state devices, or as quantum bits with dedicated configurations, as proposed for other molecular quantum bits, and in spin-based electronics.

Acc. Chem. Res. 51, 753 (2018)

Mapping and harnessing mesoscopic charge and spin textures in quantum oxide materials

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Strong electronic correlations can produce remarkable phenomena such as metal–insulator transitions[1] and greatly enhance superconductivity, thermoelectricity or optical nonlinearity. In correlated systems, spatially varying charge textures can arise at metal-insulator transitions. However, how spatially varying spin textures may influence electron transport in the presence of correlations remains unclear.

In this talk, we will report imaging experiments of the local electronic state across the metal-insulator transition of $NdNiO_3$ thin films. Both conductive atomic-force microscopy and X-ray photoemission electron microscopy reveal the nucleation of ~100-300 nm metallic domains in the insulating state, that grow and percolate as temperature increases.[2] We will discuss the transport and microscopy data within a percolation model and show preliminary results on the harnessing of this mesoscopic electronic texture in nanodevices.

In a second part, we will focus on thin films of a lightly electron-doped charge-transfer insulator, $(Ca,Ce)MnO_3$ in which we have observed a very large topological Hall effect (THE). Magnetic force microscopy reveals the presence of magnetic bubbles, whose density as a function of magnetic field peaks near the THE maximum. The THE critically depends on carrier concentration and diverges at low doping, near the metal–insulator transition.[3] We will discuss the strong amplification of the THE by correlation effects[4] and strong electron-phonon coupling.

[1] Rev. Mod. Phys. 70, 1039 (1998)
[2] Nano Lett. 18, 2226 (2018)
[3] Nature Phys. doi:10.1038/s41567 (2018)
[4] J. Phys. Soc. Japan 87, 033705 (2018)

Neutron techniques in cultural heritage

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The examination, non-destructively of medieval armour is possible by employing neutron techniques. Neutron imaging at HZB has yielded important and interesting information.

Medieval Armourers frequently placed makers marks on their products, which have become obscured over the centuries by polishing. However the strained metal below the polished surface an still affect the transmission of neutrons, and so cold neutron imaging can enable us to reconstruct the marks, without invasive techniques. Some have been revealed more successfully than others, and the reason for the different outcomes is proposed.

How the behavior of molecules in cloud droplets affect global climate

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Nano and micron-sized particles and droplets are dispersed throughout the atmosphere. These aerosols may contain both organic and mineral material, as well as water and even living organisms. Aerosols have been recognized for decades to play several key roles in Earth's climate, but still contribute the single largest source of uncertainty in our current ability to model the climate system. Despite great advances in both aerosol measurement techniques and model formulation, important gaps remain in our fundamental understanding of especially the organic aerosol fraction. This is evident in studies of e.g. new particle formation, aerosol growth and cloud activation, and atmospheric scale cloud effects, as discrepancies between experimental setups and between models and experimental results[1,2].

Over the past decade, we have explored the potential for emerging experimental methods using high-brilliance synchrotron radiation (SR) to shed light on molecular-level interactions between organic aerosol and atmospheric water. With a variety of end-station setups dedicated to studies of gasses and liquids, including supersonic liquid micro-jet, liquid flow cell, free-flying droplets and sub-2 nm molecular clusters, we have probed the molecular-level properties of atmospheric particles and droplet model systems in a variety of conditions and phase states[3,4,5,6]. Using a range of absorption, emission, and scattering based spectroscopic techniques, we have probed different aspects of structure and chemistry, focusing on the key role of aqueous organics.

Current efforts focus on enhancing the immediate atmospheric relevance of experimental design, including ambient pressures and single particle in-situ studies. We are part of the Finnish-Estonian consortium commissioning the Beamline for Atmospheric and Materials Science (FinEstBeAMS) at MAX IV Laboratory in Sweden[7]. Experimental efforts take place in parallel with ongoing model developments, to facilitate interpretation and incorporate descriptions of novel phenomena in a range of atmospheric frameworks[8].

References:
[1] Atmos. Chem. Phys. 10, 5663–5683 (2010)
[2] Geophys. Res. Lett. 39, L05802 (2012)
[3] Atmos. Chem. Phys. 12, 12227–12242 (2012)
[4] J. Phys. Chem. B 119, 4033–4040 (2015)
[5] Phys. Rev. B 95, 045402 (2017)
[6] Phys. Chem. Chem. Phys. 19, 25158-25167 (2017)
[7] Nuc. Instr. Meth. Phys. Res. A 859, 83–89 (2017)
[8] Environ. Sci.: Processes Impacts 20, 1611-1629 (2018)

Electronic properties of 2D semiconductors: from single crystals to 2D powders

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Understanding the electronic structure of transition metal dichalcogenide (TMDC) monolayers is essential for applications because the excitonic nature of TMDCs results in pronounced band gap renormalization as function of dielectric environment. We demonstrate that the band dispersion along two high symmetry directions (Γ-K and Γ-M) can be determined with angle-resolved photoemission spectra even for azimuthally disordered transition metal dichalcogenide (TMDC) monolayers, i.e., two-dimensional powders. This is enabled by selective high photoemission intensity along Γ-K and Γ-M of the single crystal band structure of four prototypical TMDCs, which singles out these features also after azimuthal integration, as done in experiment for polycrystalline monolayer samples. A robust base for investigating TMDC monolayers significantly beyond single crystal samples is thus provided.

Nickel-iron catalysts for electrochemical water oxidation – redox synergism investigated by *in-situ* X-ray spectroscopy with millisecond time resolution

Diego González-Flores[1,2], Katharina Klingan[1], Petko Chernev[1], Stefan Loos[1], Mohammad Reza Mohammadi[1], Chiara Pasquini[1], Paul Kubella[1], Ivelina Zaharieva[1], Rodney D. L. Smith[1] and Holger Dau[1]

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In future technological systems for chemical storage of renewable energy and production of non-fossil fuels, NiFe oxyhydroxides are prime candidates for efficient alkaline water oxidation (oxygen evolution reaction, OER). The synergistic effect of Ni and Fe is well documented but still insufficiently understood. Fluorescence-detected X-ray absorption spectroscopy at the K-edges of Ni and Fe provided structural information on the non-catalytic (reduced) and catalytic (oxidized) state of the NiFe catalyst. Time-resolved detection of X-ray signals during (i) cyclic voltammetry and (ii) in response to potential steps [1-3] revealed that the Ni(2+)/Ni(3+) redox transition is directly coupled to modification of the Fe ligand environment. We propose that the lattice-geometry modification of the Ni(Fe) oxyhydroxide that results from Ni oxidation enforces changes in the ligand environment of the Fe ions. The Fe sites do not undergo a distinctive redox transition, but are "enslaved" by the oxidation state changes of the Ni ions.

[1] Energy & Environmental Science 9, 2433-2443 (2016)
[2] Nature Communication 8, 2022 (2017)
[3] Sustainable Energy & Fuels 2, 1986-1994 (2018)

Samarium Hexaboride is a Trivial Surface Conductor

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Topological insulators are intriguing materials that refine the traditional distinction between metals and insulators: When the bulk electronic structure of an insulator has certain symmetry properties, its band gap must necessarily close at its surface. Following their theoretical prediction, topological insulators were established about a decade ago in materials based on the heavy pnictogens Sb and Bi and their neighboring elements; materials well captured in a single electron description.[1]

More recently interest has turned to finding systems that combine a non-trivial topology with strong electron correlation, as this may hold the key to further new phenomena. This led Dzero *et al.* to propose that the Kondo insulators, a branch of the family of heavy fermions, could be topologically non-trivial.[2] SmB_6 has widely been hailed as the first *topological* Kondo insulator after initial reports seemed to confirm this suggestion, but decisive proof is still lacking.[3] In this talk we present a compelling alternative explanation for the surface conductivity of SmB_6 based on results of high-resolution photoemission experiments.[4]

References:
[1] Journal of the Physical Society of Japan 82, 102001 (2013)
[2] Physical Review Letters 104, 106408 (2010)
[3] Philosophical Magazine 96, 3227 (2016)
[4] Nature Communications 9, 517 (2018)

J.C. Huss 06.12.18, 14:30

Climate-dependent heat-triggered opening mechanism of *Banksia* seed pods

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Fire plays an essential role in the life cycle of many plants on earth, particularly in the frequently burned regions of Australia. In order to persist in these regions, many plants rely on fire as a trigger for opening of their woody fruits, followed by seed release into an environment suitable for germination. The timed release of mature seeds from the plant canopy upon specific external stimuli is not only an important driver for vegetation dynamics in these regions, but it is also a source of inspiration for materials scientists. In this presentation, we provide insights into the seed pod structure and the properties, which govern the heat-triggered opening mechanism in the species *Banksia attenuata*. Based on a multi-scale material analysis of samples collected along a pronounced environmental gradient with decreasing rainfall and increasing fire risk, we show how one species can adjust its seed pods in order to achieve a specific opening temperature in a given region. As a conclusion from the identified features in the natural system, we deduce general principles, which might inspire the design of stimuli-responsive microstructures with 3D shape transformations.

References:
[1] Adv Sci 1700572 (2018)

Regulatory mechanisms in HECT ligases

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With an estimated 1000 members in the human proteome, the ubiquitin ligase family is the most diversified among the different classes of ubiquitination enzymes and pivotal in encoding specificity in ubiquitin signaling. The 28 ligases in the HECT family have critical roles in diverse pathophysiological settings, including cancer, cardiovascular and neurodevelopmental disorders, and infection, but are poorly characterized at the structural level. To identify gateways for specific therapeutic manipulation of HECT ligase activities it is crucial to distinguish between conserved and specific modes of regulation in this family. Here, I present our recent findings on the structural underpinnings of regulation of the HECT ligase HUWE1, a key player in tumor biology.

Abstracts of the Young Scientists Session - Neutron Day

Friday, 7th of December

Three-dimensional Laue neutron diffraction for grain mapping and reconstruction of polycrystalline materials

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The ever increasing development of new, more complex, structural and functional smart materials, has also increased the need for new advanced probing techniques that could provide information on structural properties from within a large volume of samples. Over the last few years the combination of transmission and diffraction measurements with the use of neutrons has proven to be valuable for such a task. Here we present a newly developed method for 3D grain indexing and mapping with the use of a continuous white thermal neutron beam that could potentially offer fast acquisition times and robust results. The technique is based on a simple Laue diffraction set-up that involves a two-detector system for both forward and back-diffraction. It is mainly developed for implementation at continuous neutron sources that do not necessarily have the possibility of energy-selective, wavelength resolved measurements. For the needs of the method an indexing algorithm was developed, following a forward modelling approach. First proof-of-concept experiments have been performed using the FALCON two-detector system placed at the E11 beam-port of the BER II reactor, Helmholtz-Zentrum Berlin.

Decoupled spin dynamics in the rare-earth orthoferrite YbFeO3: Evolution of magnetic excitations through the spin-reorientation transition

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Magnetic properties of spin-chain compounds with S = ½ attract a considerable attention in a modern solid-state physics. From theoretical side, they represent one of the simplest model for exploring the quantum critical behavior. However, weak perturbations to the original Hamiltonian, such as interchain interaction, exchange anisotropy and so on, which are typically unavoidable in real materials, can also induce novel exotic phenomena [1,2].
In this work, we study orthorhombic $YbFeO_3$, which is an antiferromagnet (AFM) with T_N ~ 600 K [3]. It was studied for at least 60 years due to the spontaneous spin-reorientation of the Fe subsystem, which takes a place at T_{SR} = 7.6 K, whereas Yb subsystem has no magnetic order down to at least 50 mK, and was generally considered as a paramagnetic. Here, we used a high-resolution inelastic neutron scattering spectroscopy and observed, that in contrast to this simple scenario, the spectrum of magnetic excitations consists of two collective modes well separated in energy. 3D gapped magnons with a bandwidth of ~60 meV, associated with the AFM ordered Fe subsystem, and quasi-1D AFM fluctuations of ~1 meV within the Yb subsystem, with no hybridization of those modes. Spin dynamics of the Fe could be well described in the frame of semiclassical linear spin-wave theory, but on the other hand, the rotation of the net moment of the Fe subsystem at T_{SR} drastically changes the quantum excitations of the Yb subsystem, inducing the transition between two regimes with magnon and spinon-like fluctuations. Results of the presented work show, that a weak quasi-1D coupling within the Yb subsystem, mainly neglected in previous studies, creates unusual quantum spin dynamics on the low-energy scales.

[1] PRL 101, 207201 (2008)
[2] PRL 70(23), 3651, (1993)
[3] PRB 98(6), 064424, (2018)

Crystal structure refinement of luminescent materials $NaMgH_{3-x}F_x$ by powder neutron diffraction

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Ionic metal hydrides of alkaline and earth alkaline metals are well-known to crystallise isostructurally to corresponding fluorides enabling the formation of solid state solutions.[1] For instance, representatives of the solid solution series $NaMgH_{3-x}F_x$ (x = 0, 0.5, 1, 1.5, 2, 2.5, 3) can be synthesised by solid-state reactions under hydrogen gas pressure from binary ionic hydrides, fluorides and magnesium. Rietveld refinement based on Powder x-ray diffraction data proves the $GdFeO_3$-structure type for all compounds and a trend of lattice parameters according to Vegard's law.
To determine the anion distribution, neutron diffraction data were collected for corresponding deuterides due to high incoherent scattering of neutron radiation by ^1H. The anion distribution in $NaMgD_2F$ and $NaMgD_{1.5}F_{1.5}$ was found to be statistical by Rietveld refinement based on powder neutron diffraction data collected at E9 at HZB.[2]
Alkaline and earth alkaline hydrides and fluorides have been widely examined as host lattices for photoluminescence active rare earth ions.[3] Photoluminescence measurements on europium(II) substituted $NaMgH_{3-x}F_x$ revealed a strong red shift of the emission wavelength (λem = 665 nm for $NaMgH_2F$:Eu) in comparison to violet emitting $NaMgF_3$:Eu.

[1] Phys. Chem.1993, 179, 181-185
[2] J. Solid State Chem. 2018, 258, 391-396
[3] J. Phys. Chem. C 2016, 120, 10506-10511

Entanglement in polyelectrolyte multilayers

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For many applications of polyelectrolyte multilayer (PEM) films, the mobility of the adsorbed polymers vertical to the surface is an important parameter. Studies of the internal structure of PEM films composed of various polyelectrolyte types using neutron reflectometry have revealed correlations between the strength and type of monomer-monomer interactions and layer intermixing.[1-4]
During annealing of polyelectrolyte multilayers in concentrated sodium chloride solutions (1 M NaCl) interdiffusion of polyelectrolytes occurs. We investigate the interdiffusion perpendicular to the substrate using neutron reflectivity and selectively deuterated polyanions (polystyrene sulfonate, PSS).[3,4] During build-up of polyelectrolyte multilayer films from PSS and polycation polydiallyldimethylammonium (PDADMA) the salt concentration in the deposition solution and the molecular weight of PDADMA was varied. A low salt concentration leads to stretched and flatly adsorbed chains. In contrast, high salt concentrations in the deposition solution shields the electrostatic interaction and leads to the adsorption of thicker layers and to interdigitated chains.
D(PSS), the diffusion constant of PSS, of multilayers formed at 10 mM and 200 mM NaCl can be tuned by five orders of magnitude; for both preparation conditions D(PSS) decreases exponentially with the degree of polymerization N of polycation PDADMA. Multilayers formed at 100 mM NaCl show a non-monotonic behavior. If the degree of polymerization of PDADMA exceeds the one of PSS, the diffusion constant drops suddenly by three orders of magnitude and remains low.
In summary, depending on the degree of polymerization of the polycation (PDADMA) and the salt concentration during preparation, the diffusion constant of the polyanion PSS in PDADMA/PSS multilayers can be varied by six orders of magnitude. The broad distribution of the diffusion constant is discussed in terms of prestreched polymers and polymer entanglement.

References:
[1] Science 277, 1232-1237, (1997)
[2] Macromolecules 49, 935-949, (2016)
[3] Macromolecules 45, 7995-8004, (2012)
[4] Macromolecules 48, 3983–3990, (2015)

An Assessment of Surface and Bulk Residual Stress in Selective Laser Melted Inconel 718

T. Thiede[1], S. Cabeza[1,2], T. Mishurova[1], N. Nadammal[1], A. Kromm[1], J. Bode[1], C. Haberland[3], G. Bruno[1,4]

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2 Institut Laue-Langevin, France
3 Siemens AG, Power and Gas, Germany
4 University of Potsdam, Germany

Having been introduced almost two decades ago, Additive Manufacturing (AM) of metals has become industrially viable for a large variety of applications, including aerospace, automotive and medicine. Powder bed techniques such as Selective Laser Melting (SLM) based on layer-by-layer deposition and laser melt enable numerous degrees of freedom for the geometrical design. Developing during the manufacturing process, residual stresses may limit the application of SLM parts by reducing the load bearing capacity as well as induce unwanted distortion depending on the boundary conditions specified in manufacturing.
The residual stress distribution in IN718 elongated prisms produced by SLM was studied non-destructively by means of neutron (bulk) and laboratory X-ray (surface) diffraction. The samples with different scanning strategies, i.e. hatching length, were measured in as-build condition (on a build plate) and after removal from the build plate.
The absolute values of all stress components decreased after removal from the build plate. Together with surface scan utilizing a coordinate-measuring machine (CMM), it is possible to link the stress release to the sample distortion. Obtained results indicated different residual stress states for each of the transversal, longitudinal and normal component depending on the thermal gradient in the respective direction.

In-situ analysis using neutron radiography of porous nickel materials for alkaline water electrolysis

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3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

The transition from nuclear and fossil energy to renewable energies comprises an increased demand for energy storage systems. These systems are mandatory to balance fluctuations in the energy grid, which are related to solar power and wind power. Especially hydrogen is a promising energy carrier: clean, safe and versatile. Alkaline electrolysis systems are more profitable compared to polymer electrolyte membrane electrolysis, due to that an increasing interest of this technologies is awaited from the market.[1]
In this research the focus is on the improvement of these systems by reducing the overpotential at the electrodes using new catalyst designs and enhancing the understanding of transport processes inside the electrolyte. To improve the performance of the electrolysis a fast product gas removal is essential. New catalysts consisting of nickel porous materials coated on a nickel electrode are presented.[2] The electrodes were characterized using analytical as well electrochemical tests. Furthermore, in-operando monitoring of the gas evolution was carried out using neutron radiography at CONRAD2 beamline to observe bubble formation and transport in the developed electrodes. Three-dimensional information about the electrode structure was yielded by X-ray tomography. The results obtained are used as a basis for CFD simulations. Latter allows for analysing the reactant water and gas flow within electrolysers theoretically. In particular, the simulations are focused on bubble motion inside the real micro structure of the nickel foam electrode. The comparison between the simulated 2-phase floating CFD simulation and in-situ tomography was already presented in literature.[3] Polarisation curves and the visual monitoring of the evolution and transport of the gas bubbles were used to validate the CFD model.
This work has been funded by the German Federal Ministry for Economic Affairs and Energy (BMWi Germany, project AEL3D, grant numbers 03ET6063B).

References
[1] Studie IndWEDe, BMVI (2018)
[2] Nickelelektrode, Verfahren zu deren Herstellung und deren Verwendung, E102017110863, (A1)
[3] J. Pow. Source 239, 611-622 (2013)

Comparative Microstructural Analysis of Non-Graphitic Carbons (NGCs) based on Wide-Angle X-Ray (WAXS) and Neutron (WANS) Scattering

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Non-graphitic carbons (NGCs) represent an important class of sp^2-hybridized carbon materials. They are made up of small graphene layer stacks, with the layers arranged turbostratically. The stacks are displaced and distorted to each other. Thus, NGCs lack long-range crystallographic order causing broad and overlapping scattering maxima in WAXS and WANS. Nevertheless, a quantitative description of this disordered sp^2 polyaromatic microstructure is essential to link it to macroscopic material properties.

In 2002 Ruland and Smarsly introduced a novel approach for WAXS data evaluation of NGCs. Therein the microstructure is described by up to 14 parameters, e.g. L_a (average graphene layer extent), L_c (average stack height), a_3 (average interlayer spacing) and several disorder parameters. This approach provides meaningful structural characterization of NGCs. However, the analysis of NGCs by WAXS and thus its validity generally suffers from experimental and physical limitations, e. g. damping of WAXS by the atomic form factor at large scattering vectors and incoherent scattering. Therefore, analyzing WANS data of NGCs provides fundamental advantages compared to WAXS.

In this study WANS data of several different NGC samples were acquired at the neutron scattering facility of Helmholtz-Zentrum Berlin. Data analysis was performed by fitting a theoretical scattering curve to the background-corrected WANS data using Ruland's and Smarsly's model. The analysis yielded the microstructural parameters mentioned above which were compared with the parameters obtained from WAXS data analysis. In Fig. 1 one of the obtained microstructural parameter from both WANS and WAXS data analysis is presented. This parameter as well as L_c, a_3 and the C-C bond length which are describing structural dimensions mostly overlap within their respective error margins. This proves the validity of Ruland's and Smarsly's model for analyzing the WANS data of NGCs.

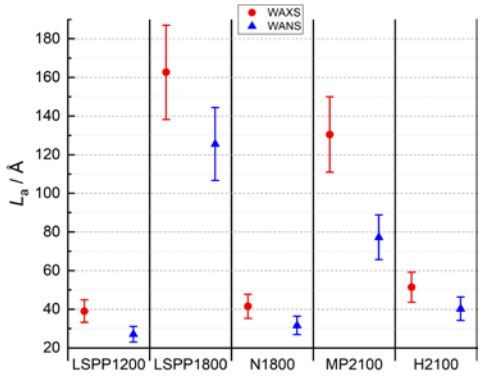


Fig. 1 Comparison of one obtained microstructural parameter (L_a, the lateral extension of graphenes) for five samples. The values mostly match within the respective error margins.
The sample precursors denoted are:
LSPP: low softening point pitch
N: Novolac resin
MP: Mesophase pitch
H: Phenol formaldehyde resin
The number indicates the heat treatment temperature in °C.

References:
[1] J Appl Cryst 35, 5, 624-633 (2002)

Poster Abstracts – Science Day at BESSY II

Thursday, 6th of December

ESUO - The European Synchrotron and FEL User Organisation: Aims and activities

Arčon I, Arikan P, Bittencourt C, Boscherini F, Braz Fernandes FM, Brooks N, Buljan M, Casu B, D'Angelo M, D'Astuto M, Feiters M, Froideval A, Gross S, Gutt C, Hase T, Huotari S, Jablonska K, Jergel M, Kajander T, Khan A, Kirm M, Kokkinidis M, Kövér L, Lamba D, Larsen HB, Lechner RT, Logan DT, López O, Lorentz K, Luning J, Mariani C, Marinkovic B, McGuinness C, Meedom Nielsen M, Mickevicius S, Mikulík P, Petukhov A, Pietsch U, Pokroy B, Purans J, Renault L, Santoro G, Shivachev B, Stangl J, Tromp M, Vankó GA, Blasetti C, Górkiewicz A, Grobosch M, Helm M, Schramm B, Seidlhofer BK, van Daalen M, Vollmer A

The European Synchrotron and free-electron laser User Organisation (ESUO) established in 2010 today represents about 30.000 users. We aim at representing the users from all European countries. Each country is represented within ESUO by one up to four national delegate(s), depending on the size of the user community in the respective country. The ESUO aims and activities are shown in this poster.

Presentation of the Lightsources.org Collaboration

Lightsources.org

Lightsources.org is the result of a collaboration between communicators from light source facilities around the world. This platform groups 22 synchrotrons and 6 FEL facilities representing 23 organisations. The website is a global resource, providing information and updates about light sources research and achievements, and opportunities for careers and international collaboration.

0a HESEB - The new Helmholtz-SESAME beamline in the soft X-ray regime

Schramm B

Starting in January 2019 five Helmholtz-Centers in close collaboration with the local staff will build a new beamline in the Soft X-ray regime (HESEB) at the SESAME synchrotron in Jordan. The construction and commissioning activities during the four years project will be accompanied by a large portfolio of training activities targeting future users.

0b Thin film processes in organic diradicals

Junghöfer T, Giangrisostomi E, Ovsyannikov R, Casu M B

We investigate chemically stable diradicals, deposited via organic molecular beam deposition in ultra-high vacuum, using X-ray Photoelectron Spectroscopy and near-edge X-ray absorption fine structure spectroscopy. Beyond the interest in organic thin films for electronics, the investigated diradicals possess a high spin (S = 1) which is of interest for novel applications in spintronics.

0c Investigation of Photochromic Molecules on Electrodes

Rhim S-Y, Ligorio G, Zorn-Morales N, Koch N, Kobin B, Hecht S, List-Kratochvil EJ

The implementation of multiple components paves the way for novel device architectures. In this contribution, we examine the switching behavior of the photochromic molecule Diarylethene on electrodes by utilizing photoemission, UV-Vis- and surface plasmon resonance spectroscopy. As a concept of proof we demonstrate the device capability of such photochromic molecules on a light emitting diode.

0d Manganese L-edge Absorption Spectroscopy on Photosystem II and Metal Complexes in Solution, using X-ray Free Electron Lasers

Kubin, Kern, Chatterjee, Gul, Fuller, Kroll, Guo, Lundberg, Odelius, Löchel, Quevedo, Erko, Föhlisch, Bergmann, Mitzner, Yachandra, Yano, Wernet

Mn L-edge X-ray absorption spectroscopy is established for photosystem II in solution and at room temperature, using an X-ray free-electron laser. Combined experimental and theoretical L-edge studies of metal complexes are used to correlate these spectra with the electronic structure of the complexes. Mechanisms and thresholds for X-ray induced sample damage are addressed.

0e Electron-electron coincidences from surfaces - The new CoESCA station at Bessy II

Leitner T, Bidermane I, Ovsyannikov R, Schumann FO, Foehlisch A, Svensson S, Martensson N

We present the CoESCA station for electron-electron coincidence spectroscopy from surfaces at the UE52-PGM beamline. It is equipped with two angular resolved time-of-flight (ArTOF) spectrometers and UHV sample preparation systems. We show first results from photoelectron - Auger electron coincidences from Ag3d, where the Auger spectra from different decay channels can be separated.

0f Magnetic and electronic properties of 3d metal benzene complexes

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

We systematically investigate the ground state of the organometallic mono- and dibenzene complexes with the 3d metals Chromium to Nickel in the gas phase in a cryogenic ion trap. By XAS we investigate the local electronic properties at the carbon and at the metal atom. Furthermore we study the magnetic properties by XMCD spectroscopy.

0g Stepwise Formation of Transition Metal Chelate Complexes

Timm M, Zamudio-Bayer V, Bülow C, von Issendorff B, Lau T

Isolated cationic transition metal chelate series are prepared by stepwise attachment of bipyridine or acetylacetonate ligands to the bare metal ion. To elucidate the nature of bonding and charge transfer, changes in the X-ray absorption spectra and core-level binding energies are monitored. The gasphase approach allows for the analysis of individual steps in the formation of the complex.

1 Ionic Current X-ray Absorption Spectra Detected in a Flow Cell

Xi L, Schellenberger M, Präg RF, Golnak R, Schuck G, Lange KM

Ionic current X-ray absorption spectroscopy (IC-XAS) relays on the synchrotron beam-induced ionization current. We investigate the mechanism by varying the spacer thickness and cell orientation. We detect Mn K-edge IC-XA spectra from several salts and study the influence of a few parameters. Potential applications and limitations are discussed.

2 Defining the phase diagram of hybrid perovskite $CH_3NH_3Pb(I_{1-x}Br_x)_3$ solid solution

Lehmann F, Franz A, Többens DM, Schorr S

Recently, hybrid perovskite materials became attractive in photovoltaic applications, offering a broad range of properties, for instance a tunable wide-bandgap, which is directly related to their chemical composition. In this poster we analyzed the $MAPbI_{3-x}Br_x$ solid solution at complete temperature range by synchrotron X-ray diffraction. As a result of this study the phase diagram was established.

3 Temperature dependence of ferroelectric phases in strained, lead-free $K_xNa_{1-x}NbO_3$ films

von Helden L, Bogula L, Hanke M Kwasniewski A, Schmdibauer M, Schwarzkopf J

$K_xNa_{1-x}NbO_3$ is a promising lead-free piezoelectric material. In thin films, its phase symmetries and transition temperatures can be modified by epitaxial strain. Here, we present temperature dependent 3D reciprocal space mappings carried out at KMC-2 beamline of BESSY II. They reveal strain induced ferroelectric phases unknown in bulk materials and significant shifts of transition temperatures.

4 Non-destructive SR-XRD characterization of surface depositions observed on ancient copper coin

Siouris IM, Katsavounis S, Emmanouilidou S, Gkirkiza MA, Litta K, Varela T, Zizak I

The diffraction profiles of coins 01, 02 and 04, are similar. Cu-alloy is the dominate phase. In contrast coin 03 shows a different profile with high Cu-Oxides concentrations. In each profile the bronze peaks shift in accordance to the Sn content.This is reflected in the variation of the crystallographic parameters. Secondary phases suggest extensive environmental interaction.

4a Advanced anomalous diffraction capabilities at KMC-2

Többens D, Zizak I, Schorr S

The monochromator of KMC-2 beamline can now be controlled directly from the diffraction endstation. This allows for seamless usage of photon energy as an adjustable parameter, extending the range of possible techniques employing anomalous diffraction. In particular, Multi Energy Diffraction Analysis (MEAD), tracking an individual Bragg peak over an absorption edge, is feasible now.

4b Cryo-EXAFS at the multi-purpose beamline KMC-2

Schuck G, Többens DM, Wallacher D, Grimm N, Schorr S

The newly build Cryo-EXAFS environment at KMC-2 XANES end station has been developed for in situ gas absorption combined with X-ray powder diffraction experiments and has been modified for use on the XANES station. With multiple Kapton windows and a variable sample holder system, experiments can be conducted in both transmission and fluorescence geometry.

5 High resolution X-ray ptychography for magnetic imaging

Bykova I, Weigand M, Keskinbora K, Sanli U, Litzius K, Gräfe J, Bechtel M, Baylan S, Richter G, Schütz G

The size of magnetic features in modern materials, i.e. domain walls or skyrmions, are scaled far below 100 nm that requires imaging with advanced resolution. X-ray ptychography is the combination of diffraction imaging and STXM that provides phase shift information and potentially wave length limited resolution. Here we present advantages of ptychography for high resolution magnetic imaging.

6 The MAXYMUS Beamline and Endstation - An Overview

Weigand M, Bykova I, Bechtel M, Gräfe J, Keskinbora K, Förster J, Simmendinger J, Stoll H, VanWaeyenberge B, Eisebitt S, Schütz G

MAXYMUS, a scanning x-ray transmission microscope (STXM), is a permanent endstation at the UE46 undulator operated by the Max Planck Institute for Intelligent Systems. We showcase endstation features like Ptychography for <10nm spatial resolution or pump and probe imaging with <20ps time resolution, as well novel STXM instrumentation like Helium cryostats or pump laser for time resolved imaging.

7 A laser for time-resolved measurements at the MAXYMUS microscope

Will I, Noll T, Weigand M, Bechtel M, Schütz G, Eisebitt S

We present a diode-pumped solid-state infrared laser installed at the MAXYMUS X-ray microscope for time-resolved pump-probe experiments. The laser produces pulses of 1 to 30 ps duration with a tuneable repetition rate between 48.7 and 50.1 MHz. This enables advanced synchronization with the filling pattern of BESSY II for pump and probe experiments with optical or thermal excitation.

10 Fluence-dependent ultrafast magnetization dynamics in TbGd bilayers and their interfacial spin-coupling

Gleich M, Bobowski K, Lawrenz D, Cagincan C, Pontius N, Schick D, Schüßler-Langeheine C, Frietsch B, Atxitia U, Thielemann-Kühn N, Weinelt M

We studied the fluence-dependent ultrafast magnetization dynamics in TbGd bilayers by XMCD in reflection. Interestingly the static magnetic properties and spin dynamics of a Gd thin film can be altered by depositing few layers of Tb on top. Our results indicate a dependency of the interfacial coupling in the TbGd bilayer on the sample temperature and a variation with distance from the interface.

13 Operando liquid electrochemistry for PEEM

Duchon T, Nemsak S, Strelcov E, Guo H, Kolmakov A, Schneider CM

We present a universal multichannel array liquid sample platform employing graphene capping that allows for investigation of interfacial liquid electrochemistry via soft X-ray absorption and photoemission spectromicroscopy. The methodology is demonstrated on copper electroplating from a buffered copper sulfate solution revealing a multi-step nucleation process at the electrified graphene membrane.

14 Photoemission electron microscopy study of MXene microflakes

Parashar B, Gospodaric P, Hantanasirisakul K, Nemsak S, Duchon T, Hackl J, Plucinski L, May S, Gogotsi Y, Schneider C

Recent advances in photoemission electron microscopy facilitate access to an electronic structure with sub-100 nm lateral resolution, either through XAS or PES. Using these techniques, we studied chemically exfoliated Ti_3C_2 MXene microflakes prepared on Si and HOPG. Isolated flakes of approx. few µm in size were characterized with their respective functional group e.g, F-, OH- and O_2- groups.

17 In-situ Low Energy Electron Microscopy at Near Ambient Pressures

Breitschaft M, Hagen S, Schaff O, Fu Q, Kampen T, Thissen A

Low-energy electron microscopy (LEEM) is a spectromicroscopy technique, which allows the study of dynamic processes at surfaces and interfaces, such as thin-film growth, surface reactions, and phase transitions. As a new development the technical capabilities of LEEM and PEEM have been extended towards near ambient conditions by developing a special objective lens concept and chamber geometry.

18 Advanced ARPES Analyzer and Momentum Microscope KREIOS 150 - Concepts and first results on layered materials and topological insulators

Wietstruk M, Dedkov Y, Fonin M, Böttcher S, Tusche C, Schönhense G, Oelsner A, Kampen T, Schaff O

Conventional ARPES analyzers only can access a limited acceptance angle and thus momentum space volume. The new KREIOS 150 Energy Analyzer uses an extractor zoom lens design to overcome these limitations. During tests at UE 56/2 (BESSY II) excellent ARPES and X-PEEM results could be obtained even on macroscopically rough surfaces or patchy samples due to its µARPES capabilities.

19 Mechanical Properties and Numerical Simulation of Nap-core Sandwich-structured Composite

Ha GX, Manfred W

Novel nap-core sandwich is studied. A two-dimensional knitted fabric is impregnated with thermosetting resin, undergoing deep-drawing and curing processes to assume a steady shape with periodic cup-shaped naps. Then, it is bonded with two thin stiff fiberglass-laminated skins to form a nap-core sandwich structure. The material is lightweight and mechanically remarkable but complex for modelling.

22 The potential of high-flux liquid anode X-ray sources for microstructure and stress analysis

Apel D, Boin M, Klaus M, Mainz R, Meixner M, Scherb T, Stange H, Wagener G, Genzel C

The two recently commissioned MetalJet stations available for external user groups as part of HZBCorelab are presented. The modular design of the stations operated at 70/160 keV and equipped with various zero/two-dimensional detectors enables in-situ/ex-situ measurements with different sample environments in angle/energy dispersive diffraction mode and simultaneous diffraction+imaging experiments.

23 Sample Environment for in situ Investigation on Nanoparticle Formation using Synchrotron X-Ray Scattering

Wendt R, Gericke E, Wallacher D, Hoell A, Rademann K, Raoux S

The developed setup facilitates in situ investigations of pressurized colloidal solutions by allowing the withdrawal of colloid solution at any time. It allows the identification and characterization of the early stages of particle formation from the molecule to final nanoparticle by simultaneous coupling of in situ UV-Vis spec., WAXS, and SAXS. The results for an NP formation are presented.

24 The EMIL Beamline(s) at BESSY-II: Status and Commissioning Results

Gorgoi M, Hendel S, Schäfers F, Gaupp A, Viefhaus J, Hävecker M, Frisch J, Lips K, Bär M, Raoux S

The EMIL beamlines use two canted undulators, UE48 and U17, to provide high brilliance across an energy range from 80 eV to 10 keV. Both undulators are now installed in the BESSY II ring. The soft and hard x-ray PGM beamlines have been well under commissioning. We will report on the energy resolution, photon flux, focus size as well as on the progress of putting the hard x-ray branch into service.

30 Band Renormalization of Blue Phosphorus on Au(111)

Golias E, Krivenkov M, Varykhalov A, Sánchez-Barriga J, Rader O

We present our results about a novel two-dimensional honeycomb lattice of phosphorus atoms, named blue phosphorus, on Au(111) surface. Using a combination of electron diffraction, scanning tunneling microscopy, theoretical calculations and angle-resolved photoemission spectroscopy we report on the structural and electronic properties of this novel phosphorus allotrope.

31 Anomalous behavior of the electronic structure of $(Bi_{1-x}In_x)_2Se_3$ across the quantum-phase transition from topological to trivial insulator

Sánchez-Barriga J, Aguilera I, Yashina LV , Tsukanova Y, Freyse F, Chaika AN, Callaert C, Abakumov AM, Hadermann J, Varykhalov A, Rienks EDL, Bihlmayer G, Blügel S, Rader O

We investigate the electronic structure of topological surface states (TSSs) across a topological quantum-phase transition. We find a surface band gap opening at the Dirac point of the TSSs, giving rise to massive fermions with non-zero spin polarization. A novel mechanism of bulk-mediated scattering processes that increase with decreasing spin-orbit coupling strength is proposed as explanation.

32 Analysis of electronic bands in metal halide perovskite single crystals via angular-resolved photoelectron spectroscopy

Sajedi, Marchenko, Krivenkov, Varykhalov, Sánchez-Barriga, Rader

Metal halide perovskite (MHP) are fascinating novel materials for future spintronics due to the strong spin orbit coupling (SOC) in their structure. Exposing (001) facets, our ARPES results of $MAPbBr_3$ and $CsPbBr_3$ single crystals reveal the 4-fold symmetry, and highly reproducible and stable parabolic dispersive features of the valence band maximum (VBM) along high symmetry surface brillouin zone.

33 Impact of Ultrafast Transport on the High-Energy states of a Photoexcited Topological Insulator

Freyse F, Battiato M, Varykhalov A, Rader O, Sánchez-Barriga J

Using trARPES we show that driving a topological insulator (TI) from the bulk-conducting into the bulk-insulating transport regime allows to selectively switch on and off the emergent channels of ultrafast transport between the surface and the bulk. We thus establish that ultrafast transport is one of the main contributions to the decay of excited electrons in prototypical TIs.

34 XPP-KMC3: The time-resolved hard X-ray diffraction endstation at BESSY II

Rössle M, Leitenberger W, Reinhardt M, Koc A, Kwamen C, Hannemann E, Bergheer M

The XPP endstation installed at the KMC3 beamline is dedicated to the investigation of the structural response of matter with ps time-resolution after either an optical laser or electrical pulse excitation of a solid state sample. We present the experimental setup and demonstrate the observed ultrafast structural response using different excitation and detection schemes available at XPP-KMC3.

35 Operando X-Ray absorption spectroscopy at metal K-edges at KMC-3 beamline: current status.

Dau H, Haumann M, Zaharieva I, Sikolenko V, Žizak I

The experimental setup of operando XAS endstation of the KMC-3 beamline is described. This station allows us to perform time resolved XAS experiment of catalyst materials in electrochemical cell. New energy-resolved 13-element Si-drift detector has been put into operation in 2018. The possibility to make XANES experiments with 1 ms time resolution has been implemented.

36 Operando studies of charge and structural motion in ferroelectric capacitors using time-resolved X-ray diffraction

Kwamen C, Rössle M, Leitenberger W, Zamponi F, Alexe M, Vilquin B, Rojo-Romeo P, Dubourdieu C, Bargheer M

We present a simultaneous study of the electrical and structural responses of lead-zirconate-titanate-based capacitor devices during charging, discharging, and polarization reversal, using time-resolved X-ray diffraction. We examine the interplay between charge flow and atomic motion in real-time. Our investigations highlight the role of the incomplete screening of the depolarization charges.

37 Structural snapshot of a bacterial phytochrome in functional intermediate states

Sauthof L, Schmidt A, Szczepek M, Fernandez Lopez M, Velazquez Escobar F, Qureshi BM, Michael N, Buhrke D, Stevens T, Kwiatkowski D, von Stetten D, Mroginski MA, Orville A, Kern JF, Krauss N, Lamparter T, Hildebrandt P, Scheerer P

Phytochromes are photoreceptors that are present in plants, bacteria and fungi. We solved several crystal structures of the phytochrome Agp2 from Agrobacterium fabrum in the parent Pfr state as well as a functional Meta-F intermediate and discuss mechanistic implications for the photoconversion.

38 Tracking the route of oxygen in a metalloenzyme by classical and serial-femtosecond crystallography

Schmidt A, Kalms J, Szczepek M, Frielingsdorf S, van der Linden P, Chatterjee R, Fuller F, Gul S, O`Riordan L, Young I, Brewster A, Sutherlin K, Butryn A, Aller P, von Stetten D, Gotthard G, Royant A, Carpentier P, Sauthof L, Kwiatkowski D, Heyder NA, Hunter M, Alonso-Mori A, Batyuk A, Utesch T, Mroginski MA, Sauter N, Yano J, Yachandra V, Orville A, Kern JF, Lenz O, Scheerer P

Hydrogenases catalyze the conversion of H_2 and are interesting in the field of renewable energy technologies. Several crystal structures of native membrane-bound [NiFe] hydrogenase of R. eutropha or with multiple reveal a fine-tuned interplay between several pathways. Serial-femtosecond crystallography as well as a soak-freeze method was used to track the route of oxygen within this metalloenzyme.

39 New insights in the structure of light-activated rhodopsin and G protein specificity

Kwiatkowski D, Heyder NA, Tiemann J, Speck D, Lê Kông K, Kleinau G, Hildebrand PW, Szczepek M, Scheerer P

Rhodopsin is a G protein coupled receptor that activates G proteins in response to light. We screened hundred crystals to solve the 1st structure of native light induced metarhodopsin II. Different G proteins are known and GPCRs can activate one or several. We present crystal structures of rhodopsin bound to Gi peptides, demonstrating conserved features in this family in comparison to others

40 Structure-based design of a light-gated proton channel

Szczepek M, Fudim R, Vierock J, Vogt A, Schmidt A, Kleinau G, Fischer P, Bartl F, Hegemann P, Scheerer P

The light-driven proton pump Coccomyxa rhodopsin (CsR) provides an unmatched opportunity to study active proton transport under controlled electrochemical conditions. In this study, the crystal structure of CsR at 2.0 Å resolution enabled us to identify unique features which guided a structure-based transformation of CsR into an operational light-gated proton channel for optogenetic applications.

46 XtalTool - the all-in-one sample holder

Feiler C, Wallacher D, Weiss MS

Cryo X-ray crystallography, used to gather spatial knowledge about biomolecules, requires several handling steps. Delicate crystals easily get disturbed during crystal harvest, cryo-protection or flash freezing. To maximize success, we have developed XtalTool / XtalTool HT as a platform supporting all steps from crystallization, ligand soaking and data collection without direct crystal handling.

46a Facilities for Macromolecular Crystallography at the HZB

Gerlach M, Feiler C, Förster R, Gless C, Hauß T, He H, Hellmig M, Kastner A, Schmuckermaier L, Steffien M, Weiss MS

The MX-group at the HZB operates three beamlines that are among the most productive MX-stations in Europe. They feature state-of-the-art experimental stations, serving 100 research groups across Europe. BL14.1 and BL14.2 are equipped with Pilatus detectors and sample changer robots, providing a high degree of automation. BL14.3 has recently been upgraded with a new microdiffractometer.

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

Hellmig M, Gerlach M, He H, Kastner A, Weiss MS

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

48 FragMAX - The MAX IV fragment screening facility

de Lima G, Mueller U

FragMAX will be a modular platform for fragment screening at MAX IV. We will create ways and means for running all constituent steps of the screening process. This includes the development and the provision of a fragment library, FragMAXlib, as well as creating the technology base for sample soak, co-crystallisation and efficient harvesting of crystals.

49 Fragment Screening on Protein Kinase A and PIM1-Kinase

Heine A, Siefker C, Klebe G

Fragment screening was performed for 2 protein kinases, PKA and PIM1, using a 361 compound library developed in our laboratory. After a thermal shift assay (TSA) prescreening, obtained hits were subjected to crystallographic screening, where a high hit rate was achieved. Results from the TSA and crystallographic screening, together with observed binding motifs for both kinases will be presented.

50 Crystallographic Fragment Screening - Workflow for Efficient User Experiments

Wollenhaupt J, Metz A, Huschmann FU, Messini N, Barthel T, Wallacher D, Wahl MC, Klebe G, Weiss MS

Crystallographic fragment screening is an established method to initiate structure-based compound development. We provide the entire workflow for efficient user experiments including fragment libraries, sample handling tools, high-throughput beamline set-ups and automated data processing. Additionally, we implemented first steps in optimization of fragment hits using diversification by catalog.

51 Structural studies on the substrate and cofactor binding modes of FAD-dependent monooxygenases

Kratky J, Weiße RH, Heine T, Tischler D, Sträter N

Styrene monooxygenases (SMOs) catalyse the enantioselective epoxidation of styrene and structurally related compounds. They are of interest for the development of new biocatalytical production processes for pharmaceuticals and fine chemicals. Our aim is to improve the substrate specificity and enantioselectivity of the SMO StyA1 for such applications.

52 Inhibition of human kallikrein 7 by coumarinic esters

Hanke S, Pippel J, Tindall CA, Ulbricht D, Heiker JT, Sträter N

Dysregulation of the protease human kallikrein7 (hK7) leads to pathophysiological inflammations in the skin. Suicide inhibitors, are developed for the treatment of hK7-associated diseases. To clarify the mode of inhibition of these compounds we used X-ray crystallography. We obtained crystals diffracting to 1.89Å and solved the first crystal structure of a kallikrein with this class of inhibitors.

53 Dose dependent data collection strategies

Taberman H, Kluza A, El Sayed O, Feiler C, Gerlach M, Weiss M

Radiation damage caused by the absorption of X-rays during the diffraction experiments remains a major challenge in macromolecular crystallography and can lead, for example, to incorrect biological conclusions. We aim to determine a dose limit crystals can be exposed to by sequential data collection on standard test crystals. The results will be used in creating a general data collection strategy.

54 Structural investigation of the mechanism of ion-independent galactooligosaccharides hydrolysis

Rutkiewicz M, Bujacz A, Bujacz G

Beta-D-galactosidase from Arthrobacter sp. 32cB is a galactooligosaccharide processing enzyme with vast application potential. Contrary to the already used in food industry galactosidases, it is able to catalyze lactose with comparative efficiency in significantly lower temperature and in ion-independent mode.

55 Liquid - Jet Photoelectron Spectroscopy of the Transition Metal Oxide Nanoparticle – Aqueous Solution Interface

Ali H, Seidel R, Pohl MN, Bergmann A, Winter B

Electronic structure of the transition metal (TM) – aqueous solution interface is crucial for enhancing the photo-electrochemical production of H_2 fuel by water dissociation. We present measurements from TM nanoparticle (NP) – water interface where we apply liquid microjet photoelectron spectroscopy. Results for several NP solutions, of different NP size and stabilizing ligands, will be reported.

56 Soft X-ray Absorption Study of Isotope Effects in Ammonia Solutions Using the Newly-developed Total-Ion-Yield Detection

Cao D, Golnak R, Schön D, Xiao J

We apply the total-ion-yield (TIY) method which was recently developed for XAS detections to the study of isotope effects in ammonia aqueous solutions. When compared to other detection methods, the TIY results show much pronounced and distinctive spectral features between the normal and deuterated samples. This study demonstrates that TIY is capable of detecting subtle effects in solutions.

57 Electrochemical Oxidation of ND-Cu_2O Electrodes probed by In-Operando X-ray Absorption Spectroscopy

Choudhury S, Kiendl B, Lounasvouri M, Hadzifejzovic EH, Ren J, Al-Temimy A, Shaker M, Tesch M, Golnak R, John F, Krueger A, Petit T

Electrochemical measurements on Cu_2O based hybrid electrodes and photocatalysts give information about the different potentials at which a change in oxidation state can be observed. Till date such a change has not been observed under in-operando conditions. Here we report the direct observation of changes in oxidation states using in-operando soft X-ray absorption spectroscopy at Cu L edge.

58 Experimental characterization of the valence electronic structure of $[Fe(bpy)_3]^{2+}$ in solution

Golnak R, Ali H, Timm M, Atak K, Lau T, Xiao J

The occupied and unoccupied valence orbitals of $[Fe(bpy)_3]^{2+}$ in aqueous solution is fully characterized by RPES and RIXS measurements at Fe L-edge and N K-edge. The valence orbitals are pinpointed in the binding energy scale through a proper energy alignment of the Fe and N spectra. The metal- and ligand-centered molecular orbitals are also identified by examining the experimental spectra.

58a Probing the absolute energetics and molecular bonding character of the MnO_4^-(aq) / MnO_4^{2-}(aq) redox pair using liquid jet photoelectron spectroscopy

Mudryk K, Seidel R, Winter B, Wilkinson I

We probed the electronic structure and molecular bonding character of the MnO_4^-/MnO_4^{2-} redox pair, determining absolute ionization potentials and assigning atomic orbital parentages. Our results allow the estimation of the reorganization energy and electron transfer rate, providing insight into the electronic charge distribution in electrochemical processes involving this highly-reversible pair.

58b Effect of Surface Chemistry on Optical, Chemical and Electronic Properties of Blue Luminescent Carbon Dots

Ren J, Weber F, Weigert F, Choudhury S, Ritter E, Bande A, Schade U , Resch-Genger U, Petit T

Carbon dots are expected to be suitable for a wide range of applications. Tuning the surface chemistry provides an efficient approach to modulate their fluorescence and electronic properties. Herein, various spectroscopies, including XAS, XES and infrared spectroscopy are employed to compare systematically the electronic and chemical structures of different surface-functionalized carbon dots.

58c Study of Electronic structure of aqueous iodine species using soft x-ray photoelectron spectroscopy (XPS) and resonant x-ray photoelectron spectroscopy (RPES)

Ahsan, Hein, Wilkinson

The surface and bulk sensitive valence and core electronic structure of different aqueous (aq.) iodine species have been probed using XPS. The study reveals different species in triiodide (aq.) solution, isolates O 1s between iodate and water and shows BE shifts among different oxidation states. O 1s RPES scans were also recorded to probe the relaxation process in aqueous iodate solutions.

58d SOL^{3}PES – a new experimental setup for liquid phase soft X-ray photoemission spectroscopy at BESSY II

Seidel R, Hein D, Wartner G, Ali H, Pohl M, Winter B

We present the experimental setup SOL^{3}PES equipped with a high-transmission hemispherical electron analyzer for soft X-ray photo- and Auger-electron spectroscopy from liquid phase that has been built for operation at BESSY II. Its name is derived from solid, solution, and solar, and refers to the aim of studying solid–liquid interfaces, optionally irradiated by photons in the solar spectrum.

58e Soft X-ray induced charge dynamics in gas phase oligonucleotides

Wang X, Li W, Douma W, Bijlsma K, Hoekstra R, Bari S, Schwob L, Schlathölter T

In biological systems, the halogenated nucleobase 5-bromouracil (BrU) can replace thymine in DNA sequences, which is regularly used as a radiosensitizer in radiotherapy. We are using BrU-containing gas-phase oligonucleotides to study migration of charge and energy in these systems. In a first series of experiments, we have studied the influence of the number of A units on the yield of G-containing fragments for various photon energies.

59a Oxygen Intercalation and Oxidation of Atomically Thin h-BN Grown on a Curved Ni Crystal

Makarova A, Fernandez L, Usachov D, Fedorov A, Bokai K, Smirnov D, Laubschat C, Vyalikh D, Schiller F, Ortega E

Using a curved Ni crystal we systematically studied the effect of thermal oxygen exposure on h-BN monolayer interfacing a full variety of vicinal orientations around the (111) high-symmetry direction. We demonstrate the occurrence of two processes upon oxygen exposure: oxygen intercalation underneath the h-BN layer and oxidation of h-BN itself, which proceeds via substitution of nitrogen atoms.

59b Interaction of graphene/Co interface with oxygen

Bokai K, Shevelev V, Marchenko D, Fedorov A, Usachov D

Performing a systematic spectroscopic and microscopic investigation we studied the interaction of molecular oxygen with polycrystalline and oriented graphene, synthesized on Co substrate. We have found that at elevated temperatures controllable etching of graphene with oxygen allows to efficiently visualize grain boundaries and defects using photoemission electron microscopy.

59 Efficiency characterization of soft x-ray varied-line-spacing gratings with low stray light at Optics Beamline Reflectometer, BESSY II Beamline

Liu Y

Soft x-ray varied-line-spacing gratings are indispensable for flat-flied spectrometers. We propose a fabrication method based on electron beam lithography (EBL) and dynamic expose near-field holography. The efficiency of gratings were characteried from 1 to 5nm. The results show that the stray light of the gratings due to the stitching error of an EBL-written mask can be significantly suppressed.

60 Metrology for High Energy Accelerator: SR at wave-length Investigations on Technical Surface

Liedl A, Angelucci M, La Francesca E, Buchheim J, Gwalt G, Sokolov A, Sertsu MG, Schäfers F, Siewert F, Cimino R

Highest energy proton circular colliders like the future circular hadron collider will emit a significant flux of SR. It is, therefore, very important to characterize reflectivity and photo yield from technical surfaces. Such material properties may trigger multi-bunch, vacuum and e-cloud related instabilities. A systematic experimental study has been performed at the Reflectometer station by HMI.

61 Femtosecond and Attosecond Electron-Transfer Dynamics in PCPDTBT and PCBM Bulk Heterojunctions

Johansson FOL, Ivanovic M, Svanström S, Cappel UB, Peisert H, Chassé T, Lindblad A

We demonstrate charge-transfer times in the femto- and attosecond regimes in blends of a low-band gap polymer (PCPDTBT) and a fullerene derivative (PCBM) using the core-hole clock method. We demonstrate that this method can give information about local electron dynamics at interfaces between constituting parts, the crucial part of a bulk heterojunction where the initial charge separation occurs.

62 Live monitoring for oxygen diffusion in $Fe_3O_4/SrTiO_3$ heterointerfaces by hard X-rays

Hamed MH, Hinz RA, Rosenberger P, Szyjka T, Duarte RF, Müller M

Oxideinterfaces reveal exciting phenomena for novel spintronic applications. Controlling the magnetic and electronic properties of $Fe_3O_4/SrTiO_3$ heterointerfaces is our mean goal. We present the impact of annealing on the oxygen diffusion through heterostructure by conducting HAXPES. An interfacial chemical transition from a ferrimagnetic Fe_2O_3 phase towards antiferromagnetic FeO phase is detected.

63 Electronic state of Sr_2FeMoO_6 thin films altered through ex-situ treatments

Angervo I, Saloaro S, Granroth S, Huhtinen H, Paturi P

We investigate the effects of various ex-situ treatments on thin films composed of a promising material candidate for spintronics, Sr_2FeMoO_6 (SFMO), with soft and hard X-ray photoelectron spectroscopy. The results are obtained with a laboratory setup of Perkin-Elmer PHI 5400 using Mg K-alpha (1253.6 eV) X-ray radiation and more profoundly with HIKE end-station of the KMC-1 beamline in BESSY II.

64 Sodium intercalation in TiO_2 electrodes during dis/charging of sodium ion batteries monitored by operando XANES measurements

Andreas S, Xinwei D, Roberto F, Bastian K, Giorgia G, Evelyn H, Regan GW, Daniel B, Garcia-Diez R, Passerini S, Bär M

We report an NEXAFS operando experiment monitoring the intercalation of Na into TiO_2 nanoparticle anodes via the Ti absorption measured through the charge collector while dis/charging the battery. Changes in the number of nearest neighbors of the Ti atom and in the Ti oxidation state from Ti^{4+} to below Ti^{3+} during sodiation were observed. The changes were only quasi-reversible during desodiation.

65 Control of the interface formation between TiN and oxides by insertion of thin oxide layer

Sakhonenkov S, Gaisin A, Konashuk A, Kasatikov S, Filatova E

The formation of an interlayer at the TiN/oxide interface was studied using HAXPES. It was established that the interface can be effectively controlled by insertion of thin layer; Al_2O_3 restricts to some extent the oxidation of TiN; the amount of TiO_2 phase can be increased or decreased during the ALD process of oxide enabling engineering of vacancy-mediated processes.

66 Effect of Sr-doping on the chemical and electronic structure of $MAPbI_3$

Félix R, Phung N, Hartmann C, Nie K, Wilks RG, Abate A, Bär M

We investigated the chemical and electronic structure of a Sr-doped $MAPbI_3$ sample series via HAXPES. The addition of Sr reduces the presence/formation of Pb(0). Surface accumulation of Sr in samples with higher Sr-doping concentrations suggests a Sr lattice incorporation saturation. The impact of these findings on the electronic structure and performance of resulting solar cells is discussed.

66a Effect of NaF and NaF/RbF post-deposition treatments on the $Cu(In,Ga)Se_2$ surface and the deeply buried $Cu(In,Ga)Se_2$ /Mo interface structure

Bombsch, Avancini, Carron, Handick, Garcia-Diez, Hartmann, Félix, Ueda, Wilks, Buecheler, Tiwari, Bär

We use hard x-ray photoelectron spectroscopy to study the impact of NaF and NaF/RbF PDTs on the chemical and electronic structure of the $Cu(In,Ga)Se_2$ (CIGSe) absorber surfaces and the deeply buried CIGSe/Mo interface, accessed by lifting the CIGSe layer off the Mo substrate. While the alkali elements are present at the CIGSe front and back surfaces, the Cu, Ga, and In composition changes.

66b Electronic Structure Study of Manganese Oxide Films on Tantalum Oxynitride Photoanodes Probed by HAXPES and ResPES

Shaker MN, Favaro M, Plate P, Irani R, Abdi F, Smirnov D, Makarova A, Klyushin A, Félix R, van de Krol R, Starr D

Combining MnO_x catalyst with TaON is a potential photoanode for water splitting. The MnO_x thickness is crucial to the activity, likely due to changes in the chemical and electronic structure at the interface. Changes in Mn oxidation state and band bending were studied via HAXPES as a function of film thickness. ResPES reveals the influence of Mn oxidation state on the Mn partial density of states.

66c Investigation of the RbF treated Cu(In,Ga)Se_2/CdS interface at the high kinetic energy photoelectron spectroscopy facility at BESSY II

Maticiuc N, Kodalle T, Ümsür B, Bertram T, Wenisch R, Wang Y, Majumdar I, Yetkin H.A, Félix R, Kaufmann C.A, Schlatmann R, Lauermann I

The high kinetic energy electron (HIKE) spectroscopy facility at BESSY in Berlin was used in this study for the investigation of Cu(In,Ga)Se_2 absorber layers with varied Cu-content before and after RbF post deposition treatment. In addition, the same RbF modification of CIGSe was analyzed before and after the interface formation with a CdS buffer layer by chemical bath deposition.

66d Ion migration in organic-inorganic hybrid perovskite solar cell absorbers under operating conditions monitored by HAXPES

Nie K, Tockhorn P, Kegelmann L, Hartmann C, Félix Duarte R, Wilks RG, Albrecht S, Bär M

The stability of perovskite solar cells is limited, and the J(V) hysteresis phenomenon is far from being fully understood. Ion migration has been suggested as a possible source of both issues. Hard x-ray photoelectron spectroscopy of a simplified device while a bias voltage is applied in situ indicates ion migration and eventually phase segregation occurs under simulated operating conditions.

67 Influence of air-annealing post-deposition treatments on the CdS/Cu(In,Ga)Se_2 interface structure

Valenta D, Yetkin HA, Kodalle T, Bombsch J, Garcia-Diez R, Hartmann C, Handick E, Wilks RG, Ueda S, Kaufmann C, Bär M

Improving the efficiency of Cu(In,Ga)Se_2 based thin-film solar cells, can be achieved by an air-annealing post-deposition treatment (PDT) after CdS buffer layer deposition. Annealing above a critical temperature, however, leads to significantly deteriorated solar cell efficiencies. We used synchrotron-based HAXPES to study CdS/CIGSe interface structure before and after air-annealing PDT at 300°C.

68 S²XAFS: A new experimental setup for time-resolved X-ray absorption fine structure spectroscopy in a 'single shot'

Kulow A, Guilherme Buzanich A, Radtke M, Reinholz U, Riesemeier H, Streli C

A newly developed EXAFS setup is presented. It enables both time- and spatially resolved EXAFS information simul-taneously in a single shot. First tests of this setup were performed at the BAMline @ BESSY-II (Berlin, Germany).

69 Synchrotron Tomography of sulfur-carbon composite materials for next gen battery application

Arlt T, Titscher P, Steckermeier D, Kwade A, Manke I

A main issue of Li-S batteries is the combination of carbon and sulfur as abundant and economic materials. To investigate these materials, synchrotron tomography was used to show the mixture within the manufactured particles. Therefore, two different process routes are investigated concerning its influence on particle structure and homogeneity of the resulting carbon-sulfur composite material.

70 3D Shape Analysis of Powder for Laser Beam Melting by Synchrotron X-ray CT

Thiede T, Mishurova T, Evsevleev S, Serrano Munoz I, Gollwitzer C, Bruno G

The quality of components made by laser beam melting additive manufacturing is naturally influenced by the quality of the powder bed. In this work, the size and shape distribution of powder particles, the particle's porosity and packing density have been investigated by of synchrotron X-ray computed tomography at the BAMline in order to assess the quality of powder bed.

71 In situ investigation of mechanochemical Knoevenagel condensations of benzaldehyde derivates

Haferkamp S, Akhmetova I, Kulla H, Rademann K, Emmerling F

Mechanochemistry is known for short reaction times, nearly quantitative conversions, and decreasing amount of solvents. Among organic syntheses, the Knoevenagel condensation is an important C-C bond forming reaction. We investigated the reaction of benzaldehyde derivates (nitro- and fluoro-derivates) with malononitrile syntheses by a combination of different in situ investigation techniques.

72 Real-time In-situ Study of Simvastatin Crystallization on Levitated Droplets

Heilmann M, Bernardes CES, Emmerling F, Minas da Piedade ME

In this contribution we describe an in-situ study of the crystallization of simvastatin in three solvents. The studies were carried out by solvent evaporation at the µSpot beamline using acoustically levitated solution droplets in combination with simultaneous X-ray diffraction, Raman spectroscopy, and imaging analysis.

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

Wagermaier W, de Falco P, Li C, Schmidt I, Schemenz V, Tang T, Fratzl P

Combining microbeam scanning SAXS/WAXS together with XRF or RAMAN at the BESSY II µSpot beamline allows (i) the position resolved characterization of structure and composition of bone, (ii) SAXS/WAXS tomography on biological materials and (iii) the investigation of bioinspired crystal calcium carbonate microlens arrays.

74 In situ investigation of mechanochemical syntheses of manganese phosphonates with N-containing ligands

Akhmetova I, Emmerling F, Roth C, Rademann K

Mechanochemistry is a versatile approach for green and fast synthesis of pure substances. The exploration of the chemistry of metal phosphonates has gained considerable interest during the last decades due to their structural diversity. We synthesized manganese phosphonates in milling reactions. The mechanochemical reactions were investigated in situ to reveal the underlying mechanisms.

75 TXRF-XANES: a unique experimental setup for chemical speciation of traces down to pg range

Guilherme Buzanich A, Witte S, Fittschen UEA, Radtke M, Reinholz U, Wobrauschek P, Streli C

An automatic sample changer chamber for Total reflection X-ray fluorescence (TXRF) and X-ray Absorption Near Edge Structure analysis (XANES) in TXRF geometry is successfully set up at the BAMline at BESSY II. TXRF-XANES on different Re species in the ng range was applied. The spectra were corrected for self-absorption of the Re and an unknown species was found to be Re in +7 oxidation state.

76 Stability of the low thermal conductivity in Fe_2TiO_5 ceramics

Chen C, Müller BR, Lebedev OI, Giovannelli F, Bruno G, Delorme F

An increase in the thermal diffusivity of Fe_2TiO_5 is observed after only three cycles of measurement. X-ray refraction shows an increase in the mean specific surface. A segregation of Ca- and F-rich nanocrystals at grain boundaries is also observed by SEM and STEM-EDX. This emphasizes the importance of precursor purity and the influence of redistribution of impurities on thermoelectric properties.

77 Microstructure of Polymer-imprinted Metal-Organic Frameworks determined by Absorption Edge Tomography

Gollwitzer C, Scholz P, Ulbricht A, Joshi Y, Weidner S

Absorption edge tomography exploits the sudden change of the attenuation coefficient across the absorption edge of an element. Here, a polymer filament embedding metal organic framework was prepared and used for 3D printing. The three-dimensional distribution of the metal organic framework embedded in the polymer was determined at the beamline BAMline with the microtomograpy setup of BAM.

78 Evidence of damage evolution during creep of Al–Mg alloy using synchrotron X-ray refraction

Müller BR, Cabeza S, Pereyra R, Fernández R, González-Doncel G, Kupsch A, Bruno G

Observation of damage accumulation during creep of Al–3.85Mg using synchrotron X-ray refraction techniques (detection of internal specific surfaces with microscopic sensitivity). A significant rise in the internal specific surface with increasing creep time was observed, providing evidence for the creation of a fine grain substructure, as predicted by the solid-state transformation creep model.

79 Investigation of Rechargeable Zn-MnO_2 Batteries with X-Ray Tomography

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

We present in-operando X-ray tomographic investigations of the charge and discharge behaviour of rechargeable Zn-MnO_2 batteries. Changes in the three-dimensional structure of the zinc anode and the MnO_2 cathode material after several charge/discharge cycles were analysed. Results are compared to the behaviour of a conventional primary cell that was also charged and discharged several times.

80 Virtual Unfolding of Folded Papyri*

Arlt T, Mahnke H-E, Baum D, Etienne M, Hege H-C, Herter F, Lindow N, Manke I, Menei E, Siopi T, Lepper V*

After having recently tested the procedure of unfolding folded papyri with vertical folding lines as in the case of the “magic fold”, we have now obtained results on unfolding ancient objects from the papyrus collection of the Musée du Louvre, département des Antiquités égyptiennes, following x-ray tomography. The objects originate from the island Elephantine near Aswan. *supported by the ERC starting grant ELEPHANTINE.

81 Multiscale imaging for alkaline water electrolysers

Arlt T, Evangelisti C, Markötter H, Liebert M, Mohseninia A, Kaczerowski J, Jörisson L, Manke I

Electrolyzers are a key factor for the energy transition from fossil to renewable energy as they are versatile converters with a wide area of application. Media transport processes are still a crucial point. Especially the sintering process of transport layers is critical since the homogeneity strongly impacts the cell performance. Multiscale imaging methods deliver valuable results.

82 Residual stress analysis in selective laser melted parts of superalloy IN718

Serrano-Munoz I, Mishurova T, Thiede T, Ulbricht A, Bode J, Kromm A, Bruno G

Selective Laser Melting (SLM) is an attractive technique for producing geometrically complex parts. However, the residual stresses (RS) induced by the manufacturing can reduce the load bearing capacity as well as induce unwanted distortion. X-Ray Diffraction experiments are performed to study the RS state and distortion of an AM IN718 material produced using three different scanning strategies.

99 Catalytic and electrocatalytic interfaces investigated by PES at atmospheric pressure

Velasco Vélez JJ, Hävecker M, Jones T, Streibel V, Teschner D, Frevel L, Mom R, Stotz E, Schlögl R, Knop-Gericke A

To close pressure gap, we developed in the pas an atmospheric pressure PES cell based on graphene. We will illustrate the operation of this setup with different examples in liquid and gas phase such as the selective hydrogenation of alkynes into alkenes-alkanes and in the characterization of electrochemical processes on electrified interfaces under aqueous conditions.

100 Notable Reactivity of Acetonitrile Towards Li_2O_2/LiO_2 Probed by NAP XPS during Li-O_2 Battery Discharge

Frolov A, Zakharchenko T, Belova A, Kapitanova O, Velasco-Velez J, Knop-Gericke A, Vyalikh D, Itkis D, Yashina L

We use NAP XPS to characterize MeCN behavior in Li-O_2 battery. We elaborated the electrochemical cell with graphene electrode and solid electrolyte with solvent vapor in gas phase. During discharge MeCN was oxidized yielding species weakly bonded to the surface. XPS of clean Li_2O_2 and LiO_2, synthesized chemically in vacuum chamber and exposed to MeCN vapors, evidences for low oxidation rate.

101 In-situ XPS and Raman measurements of silver catalysts

Klyushin AY, Frei E, Lamoth M, Zwiener L, Wang Y, Carbonio EA, Hävecker M, Knop-Gericke A, Schlögl R

In-situ measurements are important to characterize catalysts under reaction conditions. In the present work, we present systematic study of silver based catalysts by in-situ X-ray photoemission and Raman spectroscopies.

102 X-ray Studies on Electrochemical Systems - Synchrotron Methods for Energy Materials

Artur A

A set of electrochemical energy experiments is shown which takes advantage of the entire portfolio of x-ray methods at synchrotrons, including hard & soft x-ray scattering, valence band spectroscopy, for electronic structure and microstructure. Braun A: X-ray Studies on Electrochemical Systems - Synchrotron Methods for Energy Materials.

103 Co porphyrin-functionalized graphene as an efficient catalyst for CO_2 reduction reaction: An in situ near ambient pressure XPS investigation

Favaro M, Klyushin A, Hävecker M, Knop-Gericke A, van de Krol R, Bogdanoff P, Starr DE

We have used soft X-ray NAP-XPS at UE56-2/PGM-1 in the joint lab BElChem to characterize a promising CO_2RR catalyst based on a CoII porphyrin-functionalized graphene. X-ray absorption spectroscopy showed no changes in the Co oxidation state upon exposure to H_2O and CO_2. Resonant NAP-XPS at the Co L3 edge showed a decrease in states about 4 eV below the Fermi level when CO_2 and H_2O are co-dosed.

104 Oxygen interaction with h-BN on Ni(111)

Späth F, Himadri S, Düll F, Steinhauer J, Bauer U, Bachmann P, Steinrück H-P, Görling A, Papp C

In an activated adsorption process, molecular oxygen forms a molecularly bound species on a supported h-BN layer on Ni(111) at room temperature. By increasing the sample temperature to 400 K, oxygen can be intercalated under h-BN. At 600 K and higher, even the oxidation of h-BN becomes possible. The system was studied by XPS and NEXAFS.

105 Light-induced reversible switching of spiropyranes adsorbed on surfaces

Nickel F, Bernien M, Kraffert K, Krüger D, Arruda L M, Kipgen L, Miguel J, Britton A J, Kuch W

Controlling molecules in direct contact with surfaces is central to molecular electronics. N K x-ray absorption spectra of spironaphthopyran on a Bi(111) surface show that it can be transformed to merocyanine by UV radiation and back to spiropyran by temperature. A fully light-induced switching is found for spironaphthooxazine on Au(111), where the back-switching is triggered by red light.

106 X-ray resonant magnetic reflectometry (XRMR) study of the interface between ferromagnetic transition metals and MgO

Boltje DB, Ilse SE, Schütz G, Goering E

Multilayer systems of ferromagnetic transition metals and MgO attract a lot of attention in the last couple of years because of their application in MRAMs. With X-ray resonant magnetic reflectometry (XRMR) we are able to determine both chemical and magnetic depth profiles. This enables us to study properties of buried layers and especially the important magnetic properties at interfaces.

106a X-ray magnetic linear dichroism as a probe for non-collinear magnetic state

Luo C, Ryll H, Back CH, Radu F

We report on exploiting the XMLD contrast for probing the non-collinear states in DyCo and FeGd ferrimagnetic thin film. From the XMCD measurements, anomalous 'wing shape' hysteresis loops are observed slightly above their compensation temperature. This effect is assumed to be mediated by the formation of an the out-of-plane domain wall formation, which is comfirmed via XMLD measurements.

106b Observation of ferrimagnetic skyrmions in $DyCo_3$ lms

Chen K, Lott D, Luo C, Radu F

We report the observation of ferrimagnetic bubble skyrmions in $DyCo_3$ single layer, via x-ray magnetic scattering, scanning transmission x-ray microscopy and Hall transport techniques. The skyrmions are formed during the nucleation and the anihilation of the magnetic maze-like domains with an obvious topological hall effect signal.

109 The New End-station PEAXIS for RIXS and XPS Measurements at the BESSY II Synchrotron

Lieutenant K, Schulz C, Xiao J, Hofmann T, Habicht K

The electronic states determine important material properties. The end-station PEAXIS at BESSY II combines two methods in one UHV system, RIXS and XPS, for mapping of electronic states of various materials. For solid state samples, it offers continuous Q variation, temperatures of 10 - 1000 K and a resolving power of up to 10000 for photons of 200 - 1200 eV showing that PEAXIS is state-of-the-art.

112 Nanoscale NEXAFS for probing TiO_2:Eu^{+3} nanoparticles Nanothermometers for single cell temperature measurements

Bittencourt C, Garvas M, Umek P, Strancar J, Koklic T, Acosta S, Nunes LAO, Werner S, Haebel C, Guttmann P

Luminescence thermometry, has raised large interest as pathological cells are warmer than normal cells. We evaluate TiO^2 nanoparticles doped with Eu^{+3} ions (NPs) as nanothermometers. Characterization of the NPs was performed using nanoscale NEXAFS, XPS and electron microscopy. Variations in the temperature were evaluated monitoring the luminescence intensity of the 5D0-7F4 emission.

113 Status of the X-Ray Microscopy Beamline U41-PGM1-XM at BESSY II

Guttmann P, Werner S, Rehbein S, Häbel C, Schneider G

We present here the status of the U41-L06-PGM1-XM beamline. Commissioning work and first results from friendly user beamtimes confirmed the expected high performance of the new setup for X-ray microscopy studies. The setup is ready for the extension into the tender X-ray range. The UE32 under development will give access to two new important absorption edges, namely sulfur and phosphorus.

114 Combination of soft X-ray microcopy with in-situ mechanical testing to image crack propagation in microchips

Kutukova K, Liao Z, Werner S, Guttmann P, Standke Y, Gluch J, Schneider G, Zschech E

The combination of high resolution X-ray imaging with in-situ mechanical testing, particularly the application of a specially designed indenter manipulator in the full-field transmission X-ray microscope at the U41-TXM beamline of the synchrotron radiation source BESSY II is used to study the fracture behavior of microchips.

114i Core lab quantum materials

Islam N, Klemke B, Feyerherm R, Siemensmeyer K

The core lab “quantum materials” offers for external users are described: - powder and single crystal preparation, - material analysis: stoichiometry, phase purity, single crystallinity etc. - orientation, shaping and crystal mount for any experiment requirement - magnetisation, resistivity, specific heat, thermal transport as function of temperature and field.

114j BLiX - The Berlin Laboratory for innovative X-ray technologies

Mantouvalou I, Grötzsch D, Malzer W, Stiel H, Kanngießer B

BLiX is an application laboratory, where state-of-the-art X-ray methodologies are adapted to the laboratory scale including X-ray microscopy, confocal µXRF, XAFS/XES with soft/hard X-ray as well as angular resolved XRF. BLiX enlarges application fields, supports beamtime preparation, facilitates routine investigations, but also offers training and education.

114k Real-time X-ray Diffraction – from the Synchrotron to the Lab

Mainz R, Stange H, Boin M, Scherb T, Klaus M, Meixner M, Apel D, Wegener G, Becker P, Just J, Marquez-Prieto J, Unold T, Genzel C

For real-time X-ray diffraction with time resolutions in the order of seconds, synchrotron radiation used to be inevitable. With the advent of liquid-metal-jet X-ray sources, high photon fluxes are also available in the lab now - enabling XRD with time-resolutions down to the sub-second range. We present real-time studies performed at the synchrotron as well as first studies from the new lab.

115 Differential pumping unit for soft X-ray photoemission experiments under ambient pressure conditions

Grüneberger R, Thiel H, Klemke B, Wallacher D, Neeb M, Kiefer K, De Krol R, Haevecker M, Knop A

A differential pumping unit has been constructed in order to cope with a pressure difference of several orders of magnitude between an ambient- pressure photoemission chamber and the adjoining ultra-high vacuum synchrotron beamline. This pumping unit has a length of less than 0.3m and is designed to enable photoemission experiments up to 1 mbar while keeping a pressure of < 5x10^-9 mbar.

116 SECoP – the Sample Environment Communication Protocol

Wutzler F, Ekström N, Faulhaber E, Kiefer K, Klemke B, Pettersson A, Rossa L, Zolliker M

SECoP is a standard protocol for communication between sample environment equipment and experiment control software. It is intended to ease the integration of new sample environment equipment into the experiment control systems at the different scattering facilities. SECoP is inclusive, simple and self-explaining. At the HZB we developed a SECoP Library that wrap the functionality of SECoP.

117 Sample Environments for Synchrotron Radiation Experiments

Grimm N, Grüneberger R, Klemke B, Neeb M, Thiel H, Wallacher D, Kiefer K

The sample environment department is supporting the synchrotron user at BESSY II based on our knowledge and experience in providing sophisticated sample environment. Especially for research areas, where no commercial solutions are available, novel parts of sample environment equipment have been developed tailored to the needs of the users.

118 Magnetic depth profiling of Fe_3O_4 and Fe_3O_4/NiO thin films by X-Ray Resonant Magnetic Reflectivity

Pohlmann T, Wollschläger J, Eugen Weschke E, Kuepper K

Fe_3O_4 thin films are discussed as material for spintronic applications. Hence, the understanding of magnetic interface effects is of utmost importance. While x-ray magnetic circular dichroism (XMCD) is either surface or bulk sensitive, x-ray resonant magnetic reflectometry (XRMR) allows for the probing of the magnetic moment depth distribution and even of buried interfaces.

119 Evolution of cooperativity in the spin transition of iron(II) complex on a graphite surface

Kipgen L, Bernien M, Ossinger S, Nickel F, Britton AJ, Arruda LM, Naggert H, Luo C, Lotze C, Ryll H, Radu F, Schierle E, Weschke E, Tuczek F, Kuch W

The evolution of cooperativity in the thermal- and light-induced spin transition of an Fe(II)-based spin-crossover complex deposited on a highly oriented graphite surface is traced in coverages ranging from submonolayers to multilayers, using NEXAFS. Anticooperativity is observed at the submonolayer; the multilayers starting from a double-layer exhibit a distinctly cooperative spin switching.

120 Improving the performance of cobalt ferrite nanoparticles as theranostic agents by palladium decoration

Shams SF, Schmitz D, Smekhova A, Svechkina N, Ghazanfari MR, Siemensmeyer K, Tavabi AH, Dunin-Borkowski RE, Pettinger S, Westmeyer G, Schmitz-Antoniak C

Comparing bare and heterodimer Pd decorated $CoFe_2O_4$ nanoparticles with magnetometry and XMCD revealed that the total magnetic moments of Fe and Co are significantly enhanced after decoration. Considering also our results from magnetic hyperthermia and UV-vis spectroscopy measurements, a significant improvement of the heating efficiency of the nanoparticles by Pd decoration is expected.

121 Alteration of Fe magnetic polarisations and Al electronic structure in $Fe_{60}Al_{40}$ films by ion irradiation and plasma treatment

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

Magnetic polarisations of Fe and electronic structure of Al atoms in $Fe_{60}Al_{40}$ thin films have been probed by element-specific XAS and XMCD techniques to unravel changes related to the local environment of absorbers. It was shown that the structural order-disorder phase transition initiated by Ne^+ ions resulting in increased Fe polarisations can be turned back by moderate hydrogen plasma treatment.

121a Coordination symmetry and magnetism of metal ions in polyoxopalladates

Smekhova A, Izarova N, Stuckart M, Svechkina N, Shams SF, Schmitz D, Schmitz-Antoniak C

Polarization-dependent element-specific x-ray absorption was applied to study electronic and magnetic properties of metal ions in polyoxopalladates. It was confirmed that magnetism of Pd^{2+} ions in central and shell positions is determined by local symmetry while capping groups influence the reduction behaviour of central Fe^{3+} ions under hydrogen plasma treatment and the resulting magnetic moments.

121b Controlling the Verwey transition at the nanoscale

Schmitz-Antoniak C, Schmitz D, Warland A, Wende H

The spin dipole term (“Tz term”) in XMCD spectroscopy was used to study the Verwey transition in Fe_3O_4 nanoparticles: (i) its suppression by surface modifications and (ii) its revival in aged particles after hydrogen plasma treatment. The results demonstrate the importance of the electronic structure for the Verwey transition and gives an example for improving the properties of nanoscale Fe_3O_4.

122 THz-EPR@BESSY II: A Versatile Experiment for Electronic Structure Determination of High-Spin Systems with Large Zero-Field Splittings

Lohmiller T, Nehrkorn J, Holldack K, Schnegg A

The THz beamline at BESSY II offers unique possibilities for THz-EPR experiments over a wide energy range up to hundreds of cm-1 and fields up to 10 T. It is a powerful method to precisely determine very large electron spin couplings, i.e. zero-field and exchange interactions, of high-spin systems such as molecular magnets, catalysts and energy materials, enabling magneto-structural correlations.

123 UNIFIT 2019 - the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

Hesse R, Denecke R

An automatic loading of a set of data files including spectra of standard measurements, the optimized quantification with a new optional 100% normalization tool as well as the saving of all design and processing steps of the selected spectra of the standard measurement and an automatic spike correction of all loaded spectra were implemented.

124 LISE/M

Beckmann, Bischoff, Naparty, Pohl, Priebsch, Zahr

LISE a framework for experiment control systems. Putting emphasis on a modular design and based on best experiences with PXI hardware and the LabVIEW software stack, these components were chosen as a development base. In development our focus have been beamlines at the storage ring but the framework should serve as universal experiment control system.

125 Supporting Research Data Management

Görzig K

The managament of research data is one of the main tasks for the next time. The poster shows a possible data flow and the subtasks where the IT department could support instrument scientists and users.

126 "Isaac" – A modular control software both for sample environment and laboratory based experiments

Klemke B, Paeckel S, Kiefer K

We are developing a software that can be used to control sample environment equipment (SEE) and to perform laboratory experiments. It benefits from a plug-in structure which allows for a very modular system, usable on all kinds of experiments. The software is in use with several SEE on different experiments. Furthermore, an interface for an easy to use TCP/IP communication (SECoP) is integrated.

137 The HZB MX-BioLab

Gless C, Feiler C, Foerster R, Gerlach M, He H, Hellmig M, Kastner A, Kluza A, Marbina S, Rutkiewicz M, Schmuckermaier L, Steffien M, Taberman H, Wator E, Weiss M, Wilk P, Wollenhaupt J, Hauß T

The HZB MX-BioLab supports the whole workflow from gene to crystal: cell cultivation, protein purification, crystallization and sample preparation. In addition, samples for other biological investigations, e.g X-ray imaging and X-ray microscopy can be prepared. The Biolab is operated by the MX-group to support external and internal users for preparing their biological samples (safety level S1).

138 Structural studies of mutants of the NaK channel

Minniberger S, Abdolvand S, Sun H, Plested AJR

Ionotropic glutamate receptors (iGluRs) mediate fast excitatory synaptic transmission in the central nervous system. Huge progress about functional mechanisms has been made but central questions concerning ion permeation and selectivity persist. Structures of mutants of the model channel NaK mimicking GluA2 give insights into the permeation mechanism, supported by molecular dynamics simulations.

139 Structure highlights of Laboratory of Structure and Function of Biomolecules

Kolenko P, Dohnalek J

Since 2006, the Laboratory of Structure and Function of Biomolecules of the Institute of Biotechnology of the Czech Academy of Sciences has belonged to MX Bessy II users. The ease of access and high technical quality of the MX beamlines enabled us determination of protein crystal structures for a number of projects in immunology and enzymology. Selected examples are reviewed.

140 Further characterization of 17β-HSD14 by mutations

Badran MJ, Bertoletti N, Braun F, Merabet A, Keils A, Heine A, Klebe G, Marchais-Oberwinkler S

17β-Hydroxysteroid dehydrogenase type 14 (17β-HSD14) is part of the SDR (Short Chain Dehydrogenase/Reductase) family which oxidizes estradiol (E2) and 5-androstenediol (5-diol) at the 17th position using NAD^+ as a cofactor. However, the role of this enzyme in vivo is not yet clear. There are 2 natural variants of-of this protein S205 and T205

141 X-ray crystallographic structural analysis of seven disease-causing mutants of human lipoamide dehydrogenase

Szabo E, Wilk P, Mizsei R, Nagy B, Zambo Z, Bui D, Hubert A, Torocsik B, Weiss M S, Adam-Vizi V, Ambrus A

High-resolution crystal structures of the human lipoamide dehydrogenase and seven of its disease-causing mutants are reported. Based on the analyses of the mutants affecting the interface domain, the cofactor binding-domain, and the active site, individual molecular pathomechanisms are proposed for the compromised catalytic activities and altered capacities for reactive oxygen species generation.

142 Structural and Functional Analysis of the RNA Helicase HrpA

Grass LM, Wollenhaupt J, Absmeier E, Barthel T, Benamar M, Wahl MC

HrpA is a bacterial RNA helicase, which enhances antibiotics resistance in E. coli. We elucidated a crystal structure of a large N-terminal fragment of HrpA (1-783), comprising all domains necessary for RNA unwinding. Functional assays show a regulatory effect of the C-terminal part on RNA binding and unwinding that is likely triggered by intra-molecular interactions of the C- and N-terminus.

143 Competing out the enemy - efficient cryo-protection using deep eutectic solvents

Marbina S, Wator E, Feiler C, Weiss MS

Cryo protectant agents are well known in X-ray crystallography as substances used to replace water within crystals to minimize ice formation due to freezing before diffraction experiments. Each crystal system requires a proper cryo-protectant if not already known. To optimize this time consuming screening procedure, deep eutectic solvents have been tested for its potential omni-protectant habits.

144 Structural analysis of human prolidase mutations and its complexes with epidermal growth factor receptors.

Wilk P, Rutkiewicz M, Wator E, Piwowarczyk R, Uehlein M, Mueller U, Weiss MS

Prolidase is the only metalloenzyme capable of cleavage of Xaa-Pro dipeptides and loss of its catalytic activity leads to serious disorder (PD). Recently it was shown, that loss of function mutants of human prolidase can bind to ectodomain of EGFR and influence growth of various carcinomas. Here we present preliminary structural studies.

145 Crystal structures of M. truncatula omega amidase in an open active state and with an arsenic adduct in the active site

Imiolczyk B, Barciszewski J, Szpotkowski K, Jaskolski M

Omega amidase is an enzyme metabolically linked to asparagine and glutamine transamination. We determined structures of Mt amidase, with the catalytic loop in an open and closed conformation with an arsenic adduct in the active site. The protein exists as a dimer with alpha-beta-beta-alpha fold in both structures. The quaternary arrangement of the subunits is also observed in solution using SAXS.

146 Interaction of NKX2.1 with DNA

Bommer M, Heinemann U

NKX2.1 is a homeodomain transcription factor involved in the development of thyroid, brain and lung epithelium. We show the X-ray structure of the DNA binding domain of NKX2.1 binding to a DNA 12-mer containing the conserved CAAG sequence and affinity measurements using microscale thermophoresis and ITC.

147 Prototyping protein expression constructs with DNA assembly, cell-free expression, bead halo assay and FSEC

Bommer M, Heinemann U

Protein (sample) production is hard work and a source of uncertainty in MX projects. We aim to inform the process by generating prototypes from assembled standard DNA parts using a cell-free kit on a microlitre-scale. Expression, intactness, ligand binding and even size-exclusion chromatography profiles are selectively detected by fluorescence, turning sequence (ideas) into answers in days.

148 Structure of the F420-reducing [NiFe]-hydrogenase from Methanosarcina barkeri: extended electron transfer pathway with trapped Ni-SIa state

Ilina Y, Lorent C, Katz S, Shima S, Horch M, Jeoung JH, Hildebrandt P, Zebger I, Dobbek H

The crystal structure of the type 3 [NiFe]-hydrogenase from M. barkeri (FrhABG) revealed two novel elements, allowing to extend the electron transfer pathway found in the homologous FrhABG from M. marburgensis. Additionally, the combination between X-ray crystallography with vibrational (IR and RR) and EPR spectroscopy at protein crystal suggests that we captured the elusive Ni-SIa state.

149 C-Phycocyanin crystallizes in hundreds of conditions

Sarrou I, Yefanov O, Komadina D., Peard N, Chapman H

C Phycocyanin is a pigment protein complex from the light-harvesting phycobiliprotein family. We purified C PC from the cyanobacterium T.Elongatus with a novel one step purification protocol. The protein crystallizes in hundreds of conditions and various crystal morphologies. The structure of C PC is resolved but this unique property might shine light in some principles of protein crystallography.

150 New structure of peptidoglycan protease - at war with Gram-positive pathogens.

Malecki PH, Mitkowski P, Jagielska E, Sabala I

M23 metallopeptidases cleave peptidoglycans (PG), the main components of bacterial cell walls of Gram+ bacteria. Enzymes belonging to this family are consider as a novel weapon against pathogens. Herein we present the crystal structure of new peptidoglycan hydrolase and its place among other M23 members. By structural-functional analysis we would like to elucidate the mechanism of PG selectivity.

151 Exhaustive X-ray Crystallographic Screening of a Hit-Enriched 96 Fragment Library Against Diverse Targets

Magari F, Metz A, Wollenhaupt J, Huschmann F, Bertoletti N, Hassaan E, Glöckner S, Siefker C, Abazi N, Heine A, Weiss M, Klebe G

As an entry point for a direct crystallographic fragment screening and drug discovery, we compiled 96 well-suited fragments. For evaluation, we crystallographically screened this library against seven diverse targets at different conditions. We also show the potential to follow up on these fragments based on feasible growing vectors in the fragment-bound structures.

152 The mysterious red protein: structure determination of Ferredoxin from T. elongatus

Wator E, Wilk P, Komadina D, Sarrou I

Despite sophisticated protein purification protocols sometimes it happens, that the actuall crystal is formed from protein other than targeted. This is more frequent when endogenous proteins are seeked. Here we present a case of endogenous ferredoxin from cyanobacteria Thermosynechococcus elongatus.

164 Phase Transitions in SnSe investigated by Far Infrared Spectroscopy

Schade U, Puskar L, Berg M, Ritter E, Efthimiopoulos I, Marcelli A, Ortolani M, Xu W, Liu Y, Zhao L

Very recently a surpassing high thermoelectric figure of merit was reported in SnSe which makes this material very attractive for electrical energy harvesting. We followed the evolution of the low-energy phonons with doping, temperature and pressure and compare the experimental results with ab initio calculations to help understanding better the low thermal conductivity in SnSe.

164a Light-induced conformational changes of transmembrane proteins probed by tip-enhanced mid-infrared differential nanospectroscopy

Giliberti V, Polito R, Ritter E, Nucara A, Calvani P, Broser M, Hegemann P, Puskar L, Schade U, Baldassarre L, Ortolani M

We apply tip-enhanced mid-infrared absorption nanospectroscopy to investigate the light-induced conformational changes of bacteriorhodopsin at the nanoscale. Difference spectra of the protein acting as a proton pump under illumination at 565 nm are obtained on cell membrane bilayers with an area of less than 1 micron^2.

164b Impact of MOFs on proton exchange membranes, In-situ IR spectroscopy

Gorban IE, Puskar L, Soldatov MA, Ritter E

This work is based on the in situ FTIR analysis of proton-conducting Nafion films modified with various Metal-organic framework structures. This allowed us to follow the changes in the parameters of modified NAFION-MOF films on the molecular level and under controlled temperature and humidity conditions. The synthesis and analysis was carried out at the HZB at the Bessy II IRIS beamline.

164c Studying proteins in motion: First µs time-resolved mid-infrared measurements on non-cyclic systems at BESSY II

Ritter E, Puskar L, Bartl FJ, Hofmann KP, Hegemann P, Schade U

Here we present for the first time microsecond time-resolved infrared measurements of the activation of vertebrate rhodopsin, prototype of G protein coupled receptors critical to pharmacology and medicine. Measurements of such irreversible reaction cascade have now become possible with our recently developed synchrotron-based mid-infrared Single shot spectrometer at the IRIS beamline of BESSY II.

164d THz- and mid IR Fourier Transform Spectroscopy on Physical Aged Polyethylene

Beckmann J, Schade U, von der Ehe K, Jaunich K, Wolff D

THz and mid IR spectroscopy of high-molecular PE and ultra high-molecular PE reveals modifications of the molecular structure. Characteristic absorption bands can be detected which are changed if the two materials are exposed by Co60 gamma radiation up to 600 kGy and subsequently stored at an annealing temperature of 398 K until for 729 days.

173 Gram-scale production of high quality nanographene under mild conditions and doping via non-destructive covalent functionalization

Donskyi I, Guday G, Lippitz A, Adeli M; Haag R, Unger W

We report a new method for top-down one-pot, gram-scale production of high-quality nanographene from graphite under mild conditions. Nanographene sheets have very low oxygen content, comparable to that of graphene grown by chemical vapor deposition. Nanographene sheets were further covalently functionalized using non-destructive [2+1] cycloaddition reaction that left the conjugated system intact.

174 Investigation of the nanoporous gold with synchrotron-based X-ray photoelectron spectroscopy.

Hänsch M, Wang W, Graf M, Wittstock G, Nefedov A, Wöll C

Nanoporous gold is a fascinating bulk-nanostructured material. It is made up of a three-dimensional mesh of ligaments which can be between some tens of nanometers up to several micrometers. In this study synchrotron XPS measurements were used to investigate the assembly of core-shell nanoparticles by varying the excitation energy.

175 NEXAFS as a tool for the analysis of extended aromatic molecules and their interfaces

Kothe M, Breuer T, Klues M, Völkner J, Witte G

Besides the application for determining the molecular orientation, spectral features in NEXAFS data can yield detailed information on chemical changes at the interface of extended aromatic molecules. Additional combination with theoretical data (StoBe) enables understanding of NEXAFS features. In this context we show the cases of the acene-fullerene interface as well as alkanethiol-SAMs on gold.

176 Amorphous hydrogenated carbon (a-C:H) surfaces as substrate for photoinduced attachement of Ruthenium (II) bi-pyridine complexes

Rouabeh W, Schlebrowski T, Nefedov A, Wehner S, Imhof W, Fischer CB

This work reports on the results of XPS-analysis carried out at HE-SGM-beamline for a series of differently substituted Ru-complexes that are covalently linked on the surface of amorphous hydrogenated carbon (a-C:H) films, which were deposited on Si-substrates via plasma enhanced chemical vapor deposition PECVD.

176a Site-selective orbital interactions in an iron carbene photosensitizer ultrathin film

Temperton R, Rosemann N, Johansson N, Guo M, Fredin L, Prakash O, Wärnmark K, Handrup K, Uhlig J, Schnadt J, Persson P

Resonant photoelectron spectroscopy (RPES) has been combined with DFT calculations to provide an in-depth analysis of ultrathin films (sub-10 nm) of a new class of iron carbene molecular complex. This allowed us to probe specific parts of the molecule, in some cases with atomistic specificity, to study molecular orbital localisation and mixing across the complex.

177 Plasma Synthesis of Carbon Based Nanomaterials

Pattyn C, Berndt J, Strunskus T, Lecas T, Boulmer-Leborgne C, Hussain S, Ammar MR, Dias A, Tatarova E, Jagodar, A, von Wahl E, Tessier PY, Cvelbar U, Traeger F, Nefedov A, Kovacevic E

Nanomaterials were synthesized in low temperature plasmas from different types of carbon precursors (from ethanol to ethylene). Common characteristics: sp2 bonding situation, high surface area, highly oriented surfaces. All plasmas are carefully studied and well controlled. In-situ material diagnostics was accompanied with XPS and NEXAFS results obtained at HESGM beam-station.

178 Determining the transmission function for SCIENTA R3000 energy analyser at the HE-SGM beamline

Müller A, Lippitz A, Radnik J, Unger WES

The determination of the transmission function T(E) of the energy analyser is crucial for the accurate quantitative analysis in X-ray photoelectron spectroscopy. For this purpose, Au, Ag and Cu reference samples were measured at four different photon energies between 525 and 850 eV. T(E) was then estimated using the software UNIFIT 2019 by comparing photoelectron line pairs of the same element.

179 Biopolymer PHB coated with thin a-C:H layers for surface refining

Schlebrowski T, Rouabeh W, Fischer Chr B, Wehner S, Nefedov A

Increasing waste and resource problems lead to a higher demand of biodegradable polymers from renewable raw materials. A promising candidate is the biopolymer polyhydroxybutyrate (PHB). To adapt this material for different applications, it can be coated with amorphous hydrogenated carbon layers (a-C:H). Here we show a detailed surface analysis of a-C:H coatings with different thicknesses on PHB.

180 Depth-dependent quantitative analysis of model biofilms by combining laboratory- and synchrotron-based X-ray photoelectron spectroscopy

Kjærvik M, Dietrich P, Thissen A, Schwibbert K, Unger W

Synchrotron XPS in the soft-X-ray regime is suitable for the detection of light elements commonly found in biological samples. Various model systems of biofilms have been developed and characterized at synchrotron- and lab-based facilities. By obtaining the chemical composition at various information depths, the vertical distribution of iodine in an artificial biofilm have been determined.

190 Debye-Waller-factor applied to the intensity of diffraction orders from rough gratings

Fernández Herrero A, Pflüger M, Soltwisch V, Scholze F

With the shrinking dimensions of the nanostructures, the observation of the effect of the roughness over their total performance becomes more important. A set of gratings with a well defined roughness is measured using GISAXS and the impact of the roughness on the diffraction orders is analysed. We study the applicability of the well-known Debye-Waller factor as a damping factor.

191 Spatially resolved reflectometry for EUV optical components

Scholze F, Fischer A, Tagbo C, Buchholz C, Soltwisch V, Laubis C

We present our new set-ups for spatially resolved measurement of reflectance and. For the transmittance measurement we prepare a homogeneous almost parallel beam and place a CCD detector close behind the sample. For the spatial resolved reflectance measurement, the illuminated spot on the mirror under investigation is imaged with 10x magnification using a Wolter-type optic onto a CCD.

192 Size and concentration of nanoparticles in suspensions: Comparison of laboratory methods to SAXS and spICPMS

Schavkan A, Krumrey M

Concentration and surface chemistry of nanoparticles are critical to the performance of these novel materials and development of measurement approaches. The goal was to develop traceable measurement and calibration protocols for particle number concentration in liquid suspensions. A target of relative uncertainty u = 10 % was specified for spherical particles with diameters from 1 to 1000 nm.

192a Exploiting GIXRF of nanostructures for element sensitive reconstruction and near-field modeling based on finite elements

Andrle A, Soltwisch V, Hönicke P, Kayser Y, Beckhoff B, Scholze F

The goal is to establish a non-destructive method with a sensitivity to the dimensional and analytical parameters of a nano-structure. Different gratings are measured with reference-free grazing incidence X-ray fluorescence (XRF). With a Maxwell solver based on finite-elements the XRF can be calculated. The measurement results and the simulations show a sensitivity to the dimensional parameters.

192b Reconstruction of grating profiles using Grazing Incidence Small-Angle X-Ray Scattering

Pflüger M, Soltwisch V, Kline RJ, Krumrey M

New approaches are needed for the fast, non-destructive measurement of nanostructures, e.g. in the semiconductor industry. GISAXS provides surface sensitivity, but the interpretation of the scattering is complicated by multiple scattering effects. We present GISAXS measurements of a series of grating samples with different pitch errors that were introduced on purpose.

192c Characterization of artificial and aerosol nanoparticles with reference-free grazing incidence X-ray fluorescence analysis

Hönicke P, Kayser Y, Unterumsberger R, Pollakowski-Herrmann B, Beckhoff B

The reference-free synchrotron-based GIXRF methodology qualifies as a traceable reference for a quantitative characterization of both artificially fabricated nanoobjects and nanoparticles. In this work, we show the available characterization capabilities using various examples of artificially fabricated nanoparticles and –objects and of nanoparticles, which were deposited from the aerosol phase.

194 Database for optical constants and fundamental parameters at PTB

Soltwisch V, Andrle A, Kaplan G, Hönicke P, Beckhoff B, Scholze F

Scattering and absorption of photons are the basis of many scientific and industrial applications. Whether for diagnostics or functionalization and optimization of materials, the knowledge of optical constants and their fundamental parameters is of importance for a successful application. The vision is to build a European database of optical constants and fundamental parameters.

195 Vacuum-compatible hybrid photon counting pixel detector for WAXS, XRD and XRR in the tender X-ray range

Cibik L, Luethi B, Pflüger M, Schavkan A, Schreiber S, Luttkus M, Krumrey M

A vacuum-compatible hybrid pixel detector has been installed in the UHV reflectometer of the four-crystal monocromator beamline of the Physikalisch-Technische Bundesanstalt. The setup is based on the PILATUS3 100k module. The spectral response, homogeneity, angular dependence and linearity of the new detector have been investigated. First results of the performance are presented.

196 A compact and calibratable von Hamos X-Ray Spectrometer based on two full-cylinder HAPG mosaic crystals for high-resolution XES and RIXS

Holfelder I, Fliegauf R, Kayser Y, Müller M, Wansleben M, Weser J, Beckhoff B

A novel calibratable von Hamos X-ray spectrometer based on up to two full-cylinder optics enables chemical speciation of elements in an energy range from 2.4 keV up to 18 keV. Using synchrotron radiation as a tunable excitation source resonant inelastic X-ray scattering (RIXS) can be carried out. The spectrometer combines high efficiency with high spectral resolution in a compact arrangement.

196a Quantitative operando X-ray absorption investigations of dissolved polysulfides at both the cathode and anode sites of Li-S batteries

Zech C, Grätz O, Hönicke P, Kayser Y, Stamm M, Beckhoff B

To understand the time-dependent processes in batteries, it is important to evaluate them in operando mode. We successfully built an operando Lithium-Sulfur coin cell to monitor dissolved cathodic active material for different SOCs and SOHs at both the anode and cathode side with the help of X-ray absorption spectrometry and calibrated instrumentation.

196b Soft X-ray STXM with Large Solid Angle of Detection for X-ray Fluorescence

Lühl L, Andrianov K, Haidl A, Dehlinger A, Dollinger C, Dierks H, Unterumsberger R, Wansleben M, Weser J, Beckhoff B, Wilhein T, Kanngießer B

Scanning transmission X-ray microscopy (STXM) in the soft energy range, especially in combination with X-ray fluorescence detection, is becoming an increasingly important tool for life sciences. We present the new flexible AnImaX STXM-XRF microscope equipped with a large solid angle of detection enabling fast scans and first proof of principle measurements on biomedical samples done at the PTB.

196c A Portable Endstation for Analytical X-ray Microscopy

Haidl A, Andrianov K, Lühl L, Dehlinger A, Hönicke P, Unterumsberger R, Weser J, Lubeck J, Wansleben M, Meurer T, Grage J, Bauer L, Dehmelt S, Nisius T, Goetzke G, Staeck S, Kanngießer B, Beckhoff B, Wilhein T

Soft X-ray microscopy enables the investigation of research topics from life science and material science with a resolution down to the tens of nanometer range. AnImaX (Analytical Imaging with X-rays) is a portable soft X-ray microscope for use at synchrotron radiation facilities. The endstation combines fullfield microscopy and scanning transmission X-ray microscopy with fluorescence detection.

197 Applications of a compact von Hamos spectrometer based on two full-cylinder HAPG mosaic crystals

Wansleben M, Kayser Y, Holfelder I, Beckhoff B

We present first applications of a wavelength-dispersive von Hamos spectrometer based on two full-cylindrical HAPG mosaic crystals. The high energy resolution enables chemical speciation of 3d metals such as titanium by means of Kβ emission spectroscopy as well as determination of absolute emission line energies realized through a sophisticated calibration procedure.

198 Determination of the mass deposition of nanostructured Ge samples with reference-free XRF

Unterumsberger, Rainer, Seim, Christian, Hönicke, Philipp, Kayser, Yves, Wählisch, Andre, Lubeck, Janin, Beckhoff, Burkhard

For the determination of the mass deposition of nanostructured samples with reference-free XRF, the lateral dimensions of the incident beam has to be known. We present a quantification method of nanostructured Ge samples using a forward calculation with a convolution of the incident beam and a model of the sample. The measurements were performed at PTB using a novel instrumentation for nm-XRF.

199 Validation of secondary fluorescence algorithms for thin layered samples using synchrotron radiation based experiments

Wählisch A, Streeck C, Beckhoff B

We investigated the reliability of secondary fluorescence algorithms of thin layered samples in XRF analysis. Using monochromatic synchrotron radiation and the reference-free fundamental parameter approach allows for a straightforward test of consistency based on a-priori knowledge of the samples. A fully traceable uncertainty budget enables assessing the validity of the theoretical algorithms.

CR1 The surface structure of AgCu catalysts in ethylene epoxidation

Schweinar K, Beeg S, Hartwig C, Rajamathi C, Kasian O, Jones TE, Piccinin S, Prieto M, Gottlob D, Schmidt T, Raabe D, Schlögl R, Gault B, Greiner MT

The surface structure of AgCu catalysts governs its superiority in ethylene epoxidation. Here, we compare experimental data from in-situ XPEEM and LEED with previously predicted stable surface structures from ab-initio thermodynamics. A positive match demonstrates the effective union of humanistic chemical intuition with modern computational power for solving an intractably large problem.

CR2 Real time observation of water formation in confined space

Prieto MJ, Klemm HW , Xiong F, Gottlob DM, Menzel D, Schmidt T, Freund H-J

We will show results regarding the in-situ and real time study of the hydrogen oxidation in confined space under a silica bilayer with the SMART microscope, by means of micro-XPS, micro-LEED and LEEM. The reaction occurs as a front with a sudden change in contrast in LEEM. Apparent activation energies for the confined reaction were obtained and will be compared with the non-confined reaction.

CR3 Effects of electron irradiation on metal supported silica bilayers

Gottlob DM, Prieto M, Tanase L, Menzel D, Schmidt T, Freund H-J

We report on the damage induced in silica bilayers on Ru(0001) (highly ordered starting systems for model catalysis for zeolites) upon interaction with low-energy electrons under realistic conditions as a function of irradiation time and electron energy. The structural information of LEEM and LEED is combined with spectroscopic characterization by micro-XPS obtained via the SMART microscope.

CR4 Laser driven skyrmion formation

Novakovic N, Mawass M, Steigert A, Volkov O, Makarov D, Kronast F

Skyrmions are topologically stable nanoscopic magnetic particle like configurations. It appears they might be faster and smaller alternative to domain walls in the data storage application. Here we repot that laser pulses can write and destroy skyrmions. We analyse different magnetic structures in samples with and without DMI. For magnetic imaging photoemission electron microscopy was used.

Poster Abstracts - Neutron Day at BER II

Friday, 7th of December

Multiscale imaging for alkaline water electrolysers

Arlt T, Evangelisti C, Markötter H, Liebert M, Mohseninia A, Kaczerowski J, Jörisson L, Manke I

Electrolyzers are a key factor for the energy transition from fossil to renewable energy as they are versatile converters with a wide area of application. Media transport processes are still a crucial point. Especially the sintering process of transport layers is critical since the homogeneity strongly impacts the cell performance. Multiscale imaging methods deliver valuable results.

In-depth investigation of the closed porosity of glassy carbons by scattering techniques

Badaczewski, Loeh, Pfaff, Clemens, Wallacher, Smarsly

Non-graphitic carbons represent important carbon materials. Linking their intrinsic porosity to the microstructure is crucial to understand effects of different precursors and carbonization temperatures. Here, we determine different structural parameter describing the carbon microstructure and the porosity.

The Discovery of the Proton Polaron

Braun A, Chen Q

A combined study with in situ QENS, electroanalytical methods, Raman spectroscopy, diffraction and mathematical model shows that proton transport in solid electrolytes is done by a Holstein polaron: the first evidence for polaron polaron and cooperative ionic transport. Q. Chen, A. Braun, MRS Energy & Sustainability, 4, E14 (2017). A. Braun, Q. Chen, Nature Communications, 8, 15830 (2017).

Developing Key Technological and Method specific Capabilities for ESS at the V20 Testbeamline - a ToF Neutron Imaging Case Study

Kadletz PM, Arnold O, Pooley DE, Lee JWL, Morgano M, Woracek R

V20 mimics the ESS pulse structure with a double disc chopper and does further pulse shaping via a wavelength frame multiplication (WFM) chopper system. 2D-ToF-data were acquired with a newly developed GP2 imaging detector and a WFM chopper setup, allowing for investigation of WFM as function of detector pixel. The results facilitate the technical development for early successful science at ESS.

A neutron diffraction investigation on the mineralogical variations of ancient Greek ceramics during firing.

Siouris, Hoser, Emmanouilidou, Dimarchopoulou, Gkirkiza, Litta

Neutrons are used to characterize Grecian archaic pottery. The aim is to obtain data on the constituent minerals, firing temperatures, uncommon additions deposited during burial. Additional measurements were performed on misfired piece of pottery to obtained temperature dependencies of the constituent phases. The results assisted to define provenance and firing temperatures of the ceramics.

Imaging of water distribution and transport in fuel cells by means of neutron imaging

Markötter H, Manke I, Arlt T, Kardjilov N, Kätzel J, Hilger A, Haußmann J, Klages M, Mohseninia A, Kartouzian D, Wippermann K, Schröder A, Sanders T, Banhart J

The water evolution and distribution in fuel cells are studied via neutron imaging. Visualizations and Quantifications of the water amounts in the membrane electrode assembly (MEA) as well as the gas diffusion layer and channel system via radiography and tomography are presented in this poster.

Challenges in the structural characterization of $Cu_2Zn(Ge_xSi_{1-x})Se_4$

Niedenzu S, Gurieva G, Franz A, Schorr S

$Cu_2ZnSiSe_4$ and $Cu_2ZnGeSe_4$ are interesting materials for photovoltaics. They crystallize in the orthorhombic wurtz-stannite type and the tetragonal kesterite type structure, respectively. Polycrystalline samples of $Cu_2Zn(Ge_xSi_{1-x})Se_4$ (x=0-1) were grown by solid state reaction and investigated by WDX, X-ray and neutron diffraction concerning chemical composition, phase content and crystal structure.

Inelastic neutron studies on pure and Rh-doped URu_2Si_2 single crystals

Prokes K, Bartkowiak M, Liu X, Prokhnenko O, Bourdarot F, Huang Y-K, Mydosh J

The pure URu_2Si_2 is a heavy fermion system that exhibits unknown, so-called hidden order. The inelastic neutron scattering using HFM-EXED shows two signals at different Q positions that have distinct field dependences. Measurements up to 26 T were able to put the theory regarding the relation between the two signals on a more solid ground. We report also results obtained on the 8% Rh doped system.

Core lab quantum materials

Islam N, Klemke B, Feyerherm R, Siemensmeyer K

The core lab “quantum materials” offers for external users are described: - powder and single crystal preparation, - material analysis: stoichiometry, phase purity, single crystallinity etc. - orientation, shaping and crystal mount for any experiment requirement - magnetisation, resistivity, specific heat, thermal transport as function of temperature and field.

Magnetic structure and magnetotransport properties of $La_{0.7}Sr_{0.2}Mn_{1-x}NixO_3$

Bushinsky M, Efimov V, Karpinsky D, Tereshko N, Schorr S, Sikolenko V, Franz A

The compounds have been studied using neutron diffraction. The substitution of Ni for Mn has been shown to result in a decrease in the Curie temperature, wherein the spontaneous magnetization decreases to zero. The results are discussed assuming strong negative exchange interactions and the absence of ionic order. This work has been supported by grants RFBR 18-52-00020 and BRFFI F18R-159

Evolution of crystal structure and magnetic properties in $Bi_{1-x}Ba_xFe_{1-x}Ti_xO_3$ multiferroics

Karpinsky D, Latushka S, Zheludkevich D, Sikolenko V, Efimov V, Franz A

$Bi_{1-x}Ba_xFe_{1-x}Ti_xO_3$ are characterized by a number of structural and magnetic transitions. Increase in the dopant content causes the transition from the rhombohedral phase to the tetragonal via a formation of the morphotropic phase boundary characterized by pseudo-cubic structure and leads to a disruption of cycloidal modulation and provides a stabilization of collinear antiferromagnetic structure

Microstructural characterization of ancient coins from Northern-East Grecian districts of Topiros and Phillipi.

Katsavounis, Hoser, Andronis Velasco, Mertzanopoulos, Karadoulamas, Dimadis

All coins are formed out of Cu-Sn-Zn- mixture 97- 99 wt.%.Peak shifts indicate variation in the Cu/Sn composition with the Zn content ~2.5 wt.%. Coin 06 shows an increased Zn amount 12.4 wt.%, suggesting Roman provenance. Some coins contain Pb 2-3 wt.% with traces of Ni and Ag . The degree of damage and attrition is reflected in the corrosion products Cu_2O and CuCl 1.5 wt.%

New routes to quantum critical materials

Stockert O, Geibel C, Gruner T, Huesges Z, Lucas S, Kaneko K, Tsutsui S, Schmalzl K, Hoser A, Prokes K, Reehuis M, Yokaichiya F

Quantum critical points (QCPs) continue to play an important role. Central issues of our studies are nonmagnetic QCPs and how geometric frustration influences a QCP. We studied the influence of frustration in the heavy-fermion system $CePd_{1-x}Ni_xAl$, but also looked on the charge-density-wave instability in $Lu(Pt_{1-x}Pd_x)_2In$. We will present neutron diffraction experiments performed on E2, E4 and E6.

Simultaneous neutron and x-ray imaging of the rhizosphere – linking hydraulic patterns to soil microstructure

Tötzke C, Kardjilov N, Lenoir N, Tengattini A, Oswald SE

Water and nutrients uptake of plants depends on the transport properties of the soil next to the roots, the rhizosphere. The combination of neutron and X-ray tomography allows for in situ studies of root system architecture, the spatiotemporal distribution of water and the microstructure of soil. It is a unique approach to study hydraulics and microstructure of the rhizosphere simultaneously.

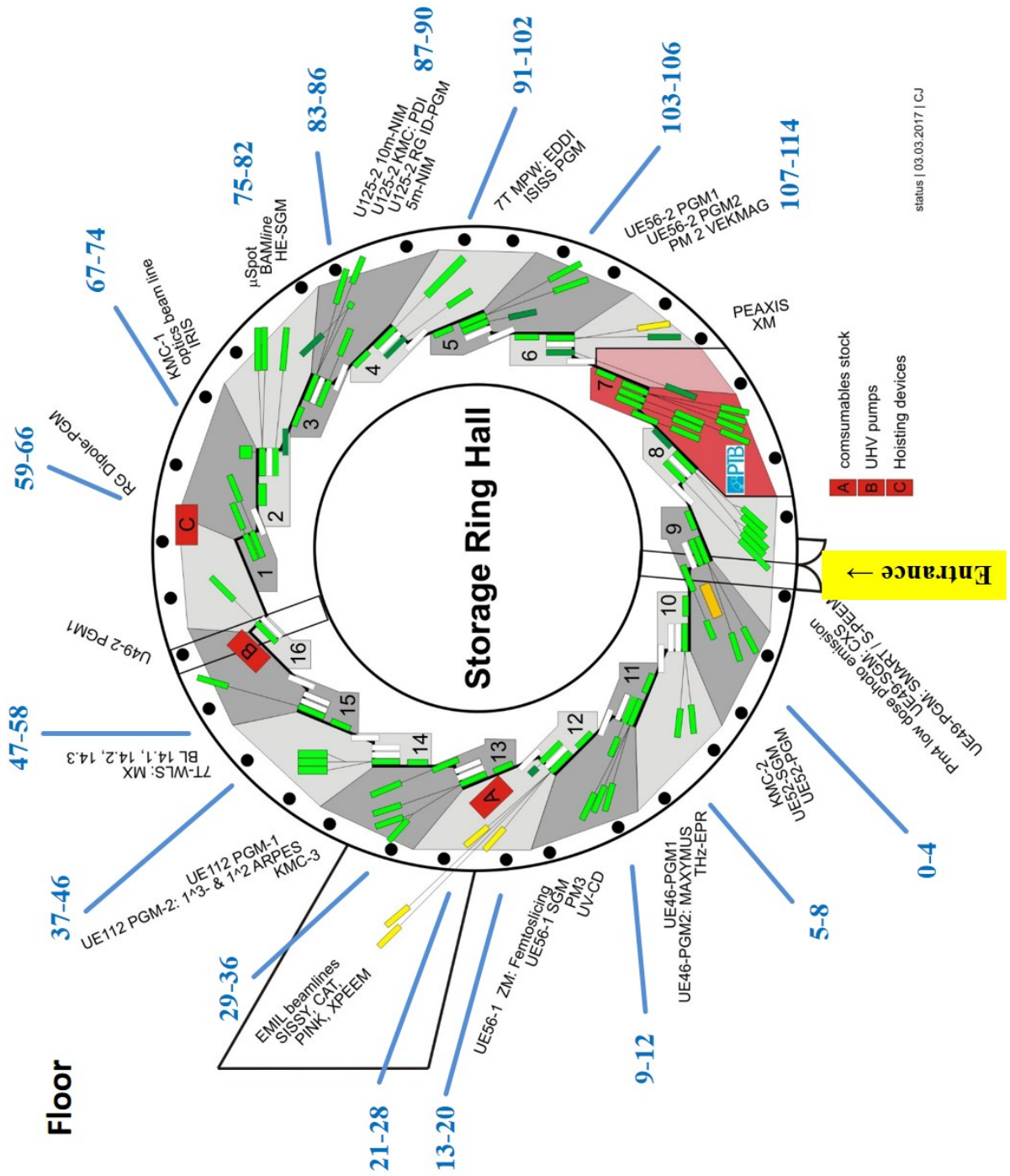
Plastic Deformation Behavior of steel measured with Neutron Imaging

Tran V K, Woracek R, Kardjilov N, Markötter H, Al-Falahat AM, Manke I, Banhart J

Plastic deformation is examined with tension experiments using varying load, and axisymmetric samples. The results show a significant dependence of plastic deformation on structure and property of the steel. The neutron radiography method is based on the variation of the transmission signal at Bragg-edges and especially useful for in-situ measurements.

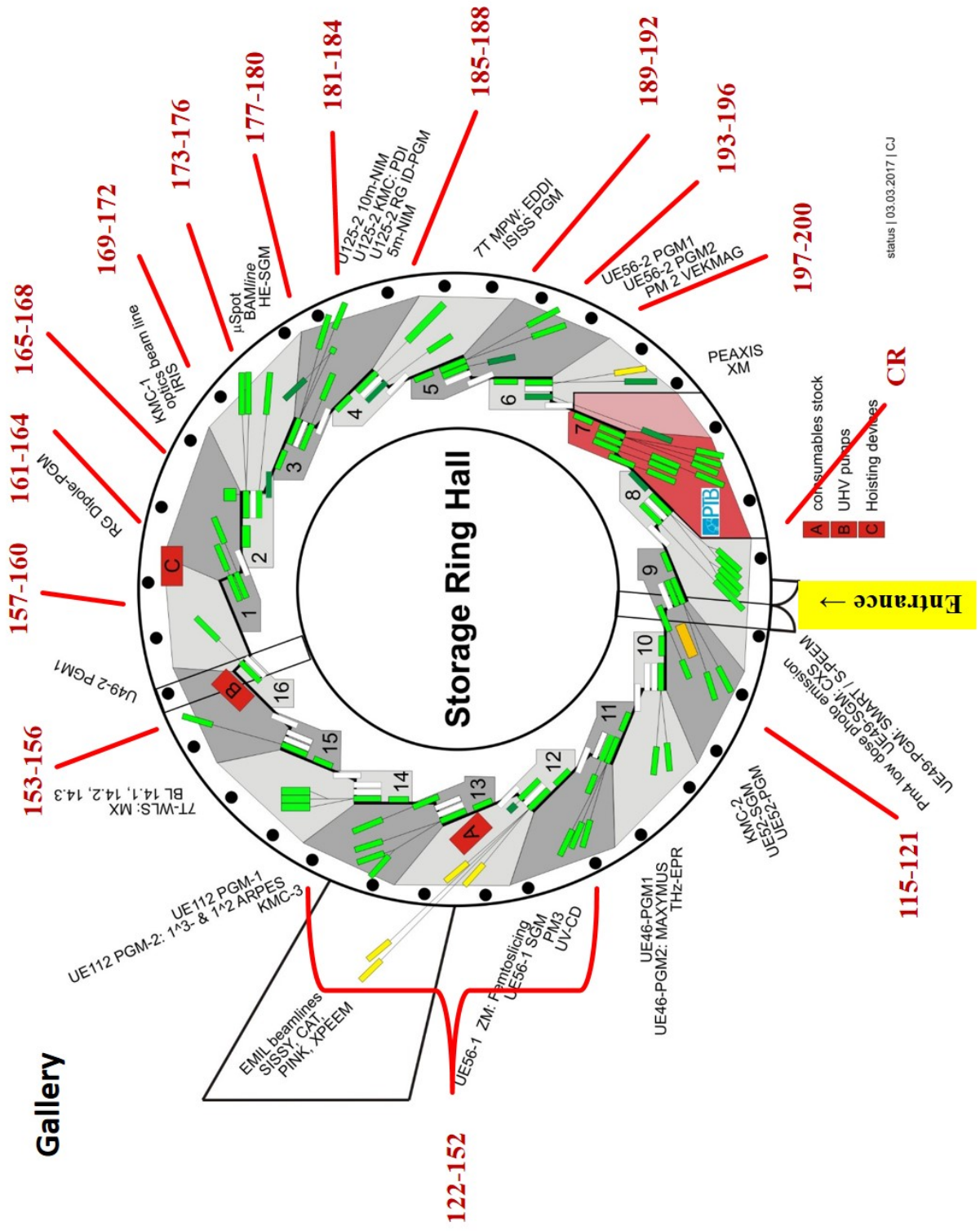
Floor Plan Poster Session – Science Day at BESSY II

Thursday, 6th of December



Floor Plan Poster Session – Science Day at BESSY II

Thursday, 6th of December



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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 2019 is
24. November 2018 [00:01] – **07. December 2018** [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 are 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

Bock-Bierbaum, Tobias	Max-Delbrück-Centrum für Molekulare Medizin, Germany	Biochemist Methods: Protein X-ray Crystallography, Structural biology Research Areas: Macromolecular complexes, biochemistry, protein structures, cancer research **Photons**
Calvet, Wolfram	TU Darmstadt	Physicist Methods: MBE, UPS, XPS, XAS Research Areas: semiconductors, photoelectrocatalysis, materials science, renewable energies, UHV **Photons**
Papp, Christian	Friedrich-Alexander-Universität Erlangen-Nürnberg, Deutschland	Chemist Methods: XPS, NEXAFS, ARPES Research Areas: Chemistry on surfaces, 2d systems, energy storage concepts **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:

Harald Schmidt	Technische Universität Clausthal	Member of the User Commitee
Olaf Schwarzkopf	HZB	Representative of the Scientific Director's Office
Beatrix-Kamelia Seidlhofer	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

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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:

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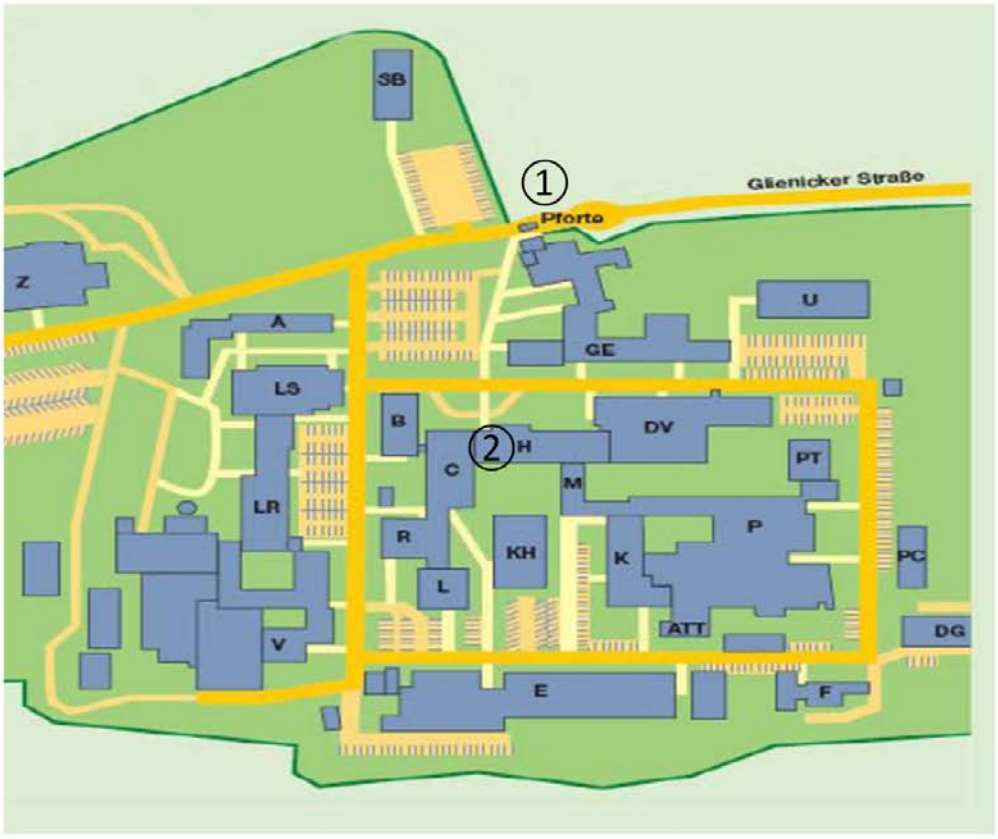
Lise-Meitner Campus
Wannsee



① Main entrance
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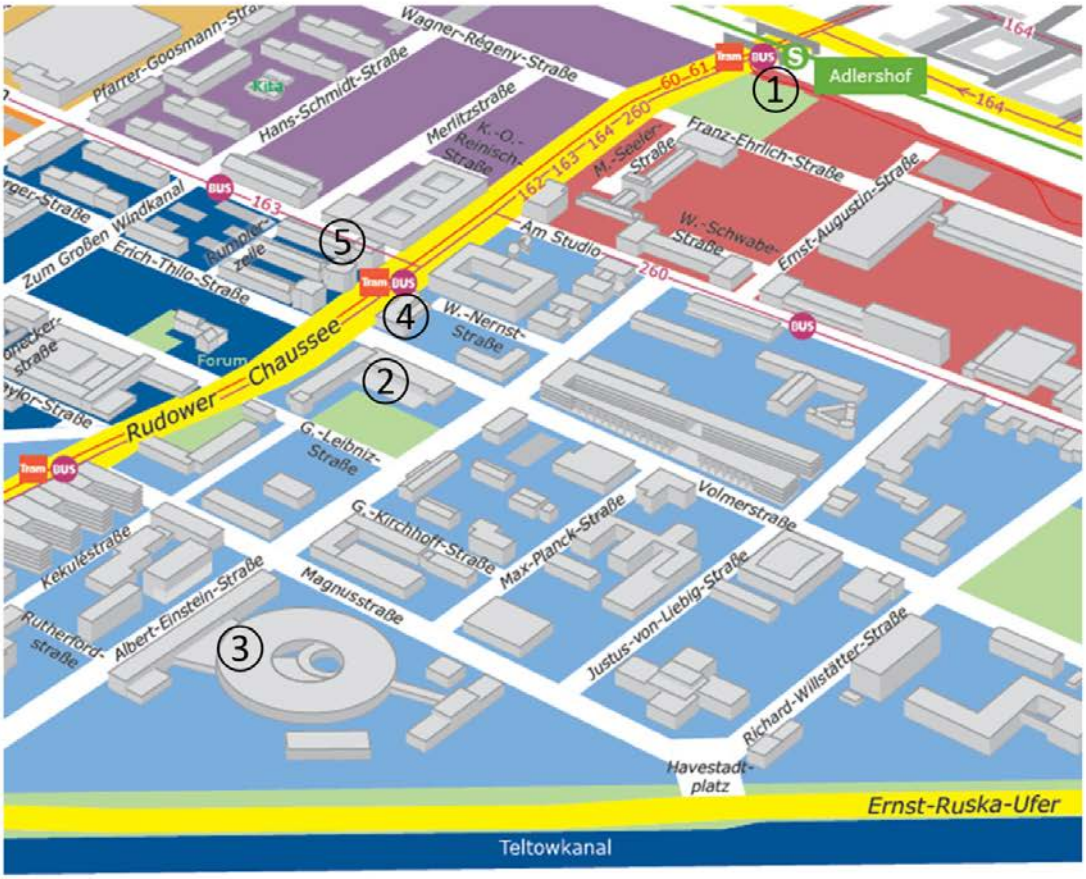

① Train Station Adlershof
② Wista centre: Registration
Bunsen Auditory
Vendor Exhibition
③ BESSY II Storage Ring Hall: Poster Session

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④ Dorint
⑤ Airporthotel

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HZB Helmholtz Zentrum Berlin

Next deadline for submission:

1st March 2019

Call for Proposals 2019/II

HZB kindly invites you to submit proposals for the next allocation period from August 2019 to February 2020 for BESSY II.

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

http://hz-b.de/gate

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

http://hz-b.de/beamguide

http://hz-b.de/proposals