HZB BESSY II Light Source

16TH BESSY@HZB USER MEETING

11 - 12 DECEMBER 2024

BESSY II & WISTA Conference Center in Berlin-Adlershof

16TH BESSY@HZB USER MEETING
COUNTRY OF HONOUR 2024: ROMANIA

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Contents

Welcome

Dear Users and Friends,

It is a great pleasure to warmly welcome you in the cooler season of the year to the 16TH BESSY@HZB User Meeting 2024. A winter meeting again, following your vote last year.

Being very successfully in operation for 26 years, BESSY II is now in the process of an up-grade called BESSY II+, which comprises novel possibilities for operando investigations, innovative new beamlines and sample environments, automation and digitalisation, storage ring improvements, and measures towards greenhouse gas neutrality of the centre. HZB is very grateful to receive significant funding from the federal government for this up-grade. This spearhead project also acts as a bridge to BESSY III, the envisioned successor source in the centre of an integrated research campus Berlin-Adlershof.

Together with our partners, mainly the PTB, MPG and BAM, universities and most importantly you, the users, we develop and realise new infrastructure, novel access modes, and integrated research opportunities jointly using synchrotron instruments, laboratories, sample environment, and off-line infrastructure in a holistic manner.

In June 2024, the Helmholtz Institute for Polymers in Energy Applications (HIPOLE) under the roof of HZB was officially inaugurated in Jena. HIPOLE is dedicated to developing sustainable polymer materials for energy technologies. In large endeavours like CatLab (Catalysis Laboratory), CARE-O-SENE (Catalyst Research for Sustainable Kerosene), GreenQUEST (German-South African initiative to develop clean household fuels), HZB contributes to solving grand challenges and empowers the research community to drive materials discovery further.

Our support for Ukraine also continues; we are coordinating partner in the “Green Deal Ukraïna” project which started in 2023 and is funded by the German Federal Ministry of Education and Research. The project aims to set up a Kyiv-based Think Tank to support Ukrainian governmental institutions, policymakers, experts, and society in making futureproof energy and climate policy decisions ahead of full EU membership.

In October a Ukrainian Synchrotron Community (USynC) has been founded. Together with Polish partners at SOLARIS, with NEPHEWS (NEutrons and PHotons Elevating Worldwide Science) and LEAPS (League of European Accelerator-based Photon Sources), BESSY II is happy to support Ukrainian user at our German-Eastern European Laboratory for Energy and Materials Research (GELEM) and builds the bridge to the Ukrainian beamline being developed at SOLARIS.

There is bad news, too, as we had a very challenging year following the cyberattack in June 2023. Although, the BESSY II storage ring was up and running again three weeks after the attack, it took time to bring all instruments back into operation. A new IT infrastructure at every beamline and a resilient network architecture had to be implemented, and the instruments gradually came back into user service. In July 2024 we were able to report that all experimental stations resumed user operation. We thank all our users for their understanding and support during this period.

After last year's very successful premiere of having a Country of Honour accompanying the user meeting (Kenya in 2023), we are happy to announce that this year’s country of honour is Romania, and we are pleased to welcome several Romanian scientists from different Romanian universities who will participate in the user meeting.

The meeting will again underline the broad variety of scientific fields addressed by the experiments realized by you at the HZB facilities. Particular highlights are the Public Lecture given by Dr. Christopher Pöhlker (Max-Planck-Institut für Chemie) on “Atmospheric Research in the Amazon: Photons, Aerosols, Clouds and a Flavor of Adventure”, the bestowal of the Ernst-Eckhard-Koch Prize for an outstanding doctoral thesis and the Innovation Award on Synchrotron Radiation as well as a “Marketplace of Innovations” which will offer time to dive deeper into several new projects at BESSY II.

We would like to thank all the vendors and companies for joining again this year and for their support of the user meeting.

We look very much forward to fruitful discussions, inspiring new ideas, a vivid exchange and future collaborations.

A cordial welcome! Enjoy the meeting!

Sincerely,

Prof. Dr. Bernd Rech	HZB User Coordination
Scientific Director	Organizing Team

Programme Day 1 / 11 December 2024 / Wednesday		
10:00 - 16:30	Vendor Exhibition (all-day alongside the meeting)	WISTA Center
09:00 - 10:00	Registration	WISTA Foyer
10:00 - 12:00	**Synchrotron Session**	**Bunsen-Hall**
10:00 - 10:05	Bernd Rech - Welcome to the User Meeting 2024	
10:05 - 10:25	Antje Vollmer - News from BESSY II and BESSY II+	
10:25 - 10:40	Markus Ries - Operation and Development of BESSY II and MLS	
10:40 - 11:00	Road to BESSY III	
11:00 - 11:15	Ruslan Ovsyannikov - Rebuilding Stronger: Post-Cyber Attack IT at BESSY II	
11:15 - 11:30	Régis Decker - X-ray emission spectroscopy using superconducting sensors	
11:30 - 11:45	Klaus Kiefer - The Future of Sample Environment at BESSY II	
11:45 - 12:00	Discussion	
12:00 - 13:00	Lunch Break	Canteens on-site
13:00 - 14:50	**Science Highlights Part I**	**Bunsen-Hall**
13:00 - 13:20	Fengli Yang (Fritz-Haber-Institut, Germany) Combining Electron and X-ray Microscopy for Operando Insights into the Evolution of Electrocatalysts Under Reaction Conditions	
13:20 - 13:40	Burak Aktekin (Justus-Liebig-Universität Giessen, Germany) Operando Photoelectron Spectroscopy Analysis of Li_6PS_5Cl Electrochemical Decomposition Reactions in Solid-State Batteries	
13:40 - 14:00	Cristian M. Teodorescu (National Institute of Materials Physics, Romania) Surface science using synchrotron radiation in the National Institute of Materials Physics, Romania	
14:00 - 14:20	Nancy Khayongo Ochiba (Technical University of Kenya) Trends in Cu-based bimetallic catalysts activity in electroreduction of carbon dioxide	
14:20 - 14:40	Hebatallah Ali (Fritz-Haber-Institut, Germany) The Metal-Oxide Nanoparticle - Aqueous Solution Interface Studied by Liquid-Microjet Photoemission	
14:40 - 14:50	Cormac Mc Guinness (Trinity College Dublin, Ireland) The European Synchrotron and FEL User Organisation (ESUO)	
14:50 - 15:20	Coffee Break	WISTA Foyer
15:20 - 16:20	**Bestowal of Prizes (EEK Prize & Innovation Award)**	**Bunsen-Hall**
16:20 - 17:20	**Science Highlights Part II**	**Bunsen-Hall**
16:20 - 16:40	Oliver Koch (Universität Münster, Germany) Fragment libraries: How sociable are they, and can we do better?	
16:40 - 17:00	Ioanna Mantouvalou (Helmholtz-Zentrum Berlin, Germany) Multimodal X-ray methods for dentistry: elemental diffusion out of fillings and into the tooth structure	
17:00 - 17:20	Christian Gutt (Universität Siegen, Germany) Committee Research with Synchrotron Radiation (KFS)	
17:20 - 17:30	Technical Break	
17:30 - 18:30	**Public Lecture**	**Bunsen-Hall**
17:30 - 18:30	Christopher Pöhlker (Max-Planck-Institut für Chemie, Germany) Atmospheric Research in the Amazon: Photons, Aerosols, Clouds and a Flavor of Adventure	
18:45	**Snacks & Beer**	**WISTA Foyer**

Programme Day 2 / 12 December 2024 / Thursday		
09:00 - 15:00	Vendor Exhibition (all-day alongside the meeting)	WISTA Center
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09:00 - 09:30	Susanne Nies (Helmholtz-Zentrum Berlin, Germany) - Green Deal Ukraine	
09:30 - 09:45	Piotr Piwowarczyk (SOLARIS, Poland) - NEutrons and PHotons Elevating Worldwide Science (NEPHEWS)	
09:45 - 10:45	**Young Scientists Session**	**Bunsen-Hall**
09:45 - 10:00	Lisa-Marie Kern (Max-Born-Institut, Germany) Imaging Nanometer Scale Spin Textures and Their Picosecond Dynamics	
10:00 - 10:15	Andrii Kuibarov (IFW Dresden, Germany) Evidence of superconducting Fermi Arcs	
10:15 - 10:30	Maximilian Mattern (Max-Born-Institut, Germany) KMC-3 XPP Accelerating the laser-induced phase transition in nanostructured FeRh via Plasmonic Absorption	
10:30 - 10:45	Evangelia Nathanail (Max Delbrück Center, Germany) Integrative structural biology to explore mitochondrial architecture	
10:45 - 11:00	Alina Marinela Badea (National Institute of Materials Physics, Romania) Vortex dynamics in high temperature superconductors	
11:00 - 11:30	Coffee Break	WISTA Foyer
11:30 - 12:30	**Science Highlights Part III**	**Bunsen-Hall**
11:30 - 11:50	Miguel Angel Valbuena (IMDEA Nanoscience, Spain) Rashba-like Spin Textures in Graphene Promoted by Ferromagnet-Mediated Electronic Hybridization with a Heavy Metal	
11:50 - 12:10	Luca Jovine (Karolinska Institute, Sweden) Mechanism of mammalian egg coat hardening and slow block to polyspermy	
12:10 - 12:30	Marcel Risch (Helmholtz-Zentrum Berlin, Germany) Understanding the electrocatalyst lanthanum nickelate by combining X-ray absorption spectroscopy and density functional theory	
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13:30 - 13:50	Hendrik Bluhm (Fritz-Haber-Institut, Germany) Multimodal Investigations of Heterogeneous Interfaces	
13:50 - 14:10	Arsène Chemin (Helmholtz-Zentrum Berlin, Germany) Understanding the Photo Electrochemistry of Diamond Water Interfaces	
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14:30 - 14:50	Gert Weber (Helmholtz-Zentrum Berlin, Germany) Enzymes for a sustainable plastic waste management	
14:50 - 15:00	Justin Wells (University of Oslo, Norway) News from the HZB User Committee	
15:00 - 15:30	Change of Location to BESSY II	
15:30 - 17:00	**Market Place of Innovations**	**BESSY Lecture Hall**
17:00 - 19:00	**Poster Session**	**BESSY Exp. Hall**
19:00	**Green Buffet**	**BESSY Foyer**

Abstracts of the Session - Science Highlights Part I

Wednesday, 11 December 2024 from 13:00 to 14:50

Bunsen-Hall at WISTA Event Center

Operando Photoelectron Spectroscopy Analysis of Li_6PS_5Cl Electrochemical Decomposition Reactions in Solid-State Batteries

Burak Aktekin[1,2], Elmar Kataev[3,4], Luise M. Riegger[1,2], Raul Garcia-Diez[3,4], Zora Chalkley[3,4], Juri Becker, Regan G. Wilks[3,4], Anja Henss[1,2], Marcus Bär[3,4,5,6], and Jürgen Janek[1,2]

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Most solid electrolytes (SEs) which are promising for all-solid-state battery (ASSB) applications are known to have a narrow electrochemical stability window.[1] Consequently, parasitic electrolyte side reactions are observed when high-energy-density electrode materials (such as lithium metal anode) are employed.[2] Therefore, it is important to determine at which potentials such reactions initiate, and which chemical species are formed as decomposition products (leading to solid electrolyte interphase, SEI). In this study,[3] a new operando experimental approach is introduced to investigate such reactions by employing photoelectron spectroscopy with hard X-rays. This experimental approach allows us to investigate SEI buried under a thin metal film (e.g., 6 nm nickel, which is partially transparent to electrons) acting as the working electrode. The feasibility of this approach is demonstrated using sulfide-based Li_6PS_5Cl solid electrolyte. The experiments show that side reactions already start at 1.75 V (vs Li^+/Li) resulting in considerable Li_2S formation, particularly in the voltage range 1.5–1.0 V. A heterogeneous/layered microstructure of the SEI is observed (e.g., preferential Li_2O and Li_2S deposits near the current collector). The reversibility of side reactions is also observed, as Li_2O and Li_2S decompose in the 2–4 V potential window, generating oxidized sulfur species, sulfites, and sulfates. The experimental approach holds promise to spectroscopically investigate electrolyte decomposition reactions under dynamic conditions for various solid electrolyte and current collector combinations.

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Surface science using synchrotron radiation in the National Institute of Materials Physics, Romania

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Surface science needs a consistent amount of funds. This area was then weakly represented in Romania prior to the admission in the European Union in 2007. An old X-ray photoelectron spectroscopy (XPS) machine donated by KU Leuven allowed the development of the necessary competences in this field from 2001. But only starting with 2008–2009 were 'real' surface science experiments set up, including preparation facilities by molecular beam epitaxy (MBE), *in situ* characterization by electron diffraction (LEED, RHEED), scanning tunneling microscopy (STM), noncontact atomic force microscopy (ncAFM), and diversification of photoelectron spectroscopy techniques including angle-resolved photoemission (ARPES) and spin-resolved photoemission. The NIMP Surface and Interface Science group employs currently 20 scientists and uses several facilities: (i) CoSMoS (combined spectroscopy and microscopy on surfaces) includes MBE, photoemission with spin resolution and STM and is installed on the beamtime SuperESCA at the Elettra synchrotron radiation facility in Trieste; (ii) a similar setup without spin resolution, provided with ncAFM together with STM; (iii) a high-throughput XPS setup, *in situ* connected to a catalytic cell working at high pressure and temperature; (iv) a low energy and photoemission electron microscope (LEEM–PEEM); (v) a laboratory X-ray absorption fine structure (XAFS) setup; (vi) a magneto-optical Kerr effect (MOKE) microscope. Setups (ii–vi) are all located in NIMP. The group collaborates with other groups from NIMP, especially by using thin films prepared by pulsed laser deposition (PLD), characterizations by X-ray diffraction and reflectometry (XRD, XRR), scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), Raman and infrared spectroscopy, cleanroom facilities etc. Synchrotron radiation activities of the group exceed the CoSMoS collaboration with Elettra, it encompasses also activities at SLS Villigen, Bessy Berlin and Soleil Saint-Aubin. A short survey of the main results obtained during the last decade will be given, including (i) works on graphene on ferroelectrics: XPS, STM and *in situ* electrical conduction as function of the substrate polarization [1,2]; (ii) molecular insertion between graphene and the underlying metal substrate [3]; (iii) molecular adsorption/desorption on ferroelectric surfaces [4–8]; (iv) surface spin asymmetry in Pt(001) [9]; (v) spin asymmetry in $SrTiO_3$(001) [10] and $SrTiO_3$(011) [11]; (vi) experimental band structure of ferroelectric thin films [12]; (vii) photoelectron spectro-microscopy on ferroelectric surfaces [13–16].

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Trends in Cu-based bimetallic catalysts activity in electroreduction of carbon dioxide

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The combustion of fossil fuels stands as a dominant contributor, responsible for approximately 75 – 80% of global greenhouse gas (GHG) emissions. These emissions are significant catalysts for the escalating global temperatures, precipitating adverse climate shifts. While the integration of renewable energy sources like solar, wind, and hydroelectric power shows promising results in mitigating GHG emissions, there is a persistent challenge in effective storage of the renewable energy. Consequently, renewable energy can be channelled into the production of sustainable fuels which offer a pathway to convert renewable energy into chemical energy compatible with existing infrastructures. Nonetheless, the electrocatalytic synthesis of synthetic fuels presents multifaceted challenges, encompassing poor product selectivity, catalyst inefficiency, and stability issues. Despite the efficacy demonstrated by precious metals, their scarcity and cost impose constraints. Present research initiatives are focused on investigating bimetallic catalysts derived from abundant earth metals, which offer affordability and the potential for enhanced selectivity, activity, and stability. This research is focussed on investigating catalytic activity trends of various Cu based bimetallic catalysts in electrocatalytic reduction of CO_2. The Cu-based bimetallic (CuM where M is Co, Fe) catalysts have been synthesized via microwave approach, characterized using different techniques e.g. XRD, XPS, SEM) and used in CO_2 reduction, in a proton exchange membrane (PEM). The catalysts have shown robust activity in CO_2 reduction and products formed include formaldehyde, methane, and ethane.

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The Metal-Oxide Nanoparticle–Aqueous Solution Interface Studied by Liquid-Microjet Photoemission

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The combination of the liquid microjet (LJ) technology and soft X-ray photoelectron spectroscopy (PES) has proven to be a highly valuable method for investigating the electronic structure of liquid water, various solvents, solutes, and nanoparticle (NP) suspensions. This experimental approach, first introduced at the BESSY II synchrotron radiation facility two decades ago, will be also greatly valuable for studying the solid–liquid interface, to identify interfacial species based on their distinctive photoelectron spectra.[1] Currently the use of PES for probing the solid–water interface is limited due to the short (inelastic) mean free path (IMFP) of photoelectrons in condensed matter, although several techniques have been developed to address this issue to some extent[2].We have yet taken another path, where we mimic the solid – water interface by the NP–water system. In that case the NPs are fully surrounded by the aqueous solution, allowing for accurate pH adjustment, and providing an environment for proton migration. Our findings on transition-metal oxide (TMO) NPs dispersed in aqueous solutions, and particle sizes smaller than the IMFP, are positioned sufficiently close to the solution–vacuum interface. Therefore, photoelectrons can be detected from both the NP–solution interface and the NP interior.[3]

We have focused on the aqueous-phase TMO NPs hematite (α-Fe_2O_3, iron(III) oxide)[4] and anatase (TiO_2, titanium(IV) oxide),[5,6] which hold great promise for applications in (photo)electrocatalysis, such as solar fuel production. A major goal is to determine how water molecules interact with the surface of these TMO NPs. We demonstrated LJ-PES's sensitivity to distinguish between water molecules in the bulk solution and those adsorbed at the NP surfaces. Additionally, we identified hydroxyl species at the NP surface, formed through dissociative water adsorption. More specifically, water is found to dissociatively adsorb at hematite NP surfaces but adsorbs molecularly at TiO_2 NP surfaces at low pH. At near-basic pH, water adsorbs dissociatively on the TiO_2 NP surface. These LJ-PES experiments also underscore the multifaceted nature of photoemission required for a comprehensive analysis of TMO NP surfaces in aqueous environments. For instance, we enhance electron signals from specific species through resonant photoemission and utilize partial electron yield X-ray absorption (PEY-XA) spectra, valence photoelectron spectra, and resonant Auger-electron spectra. We also explore the potential of these resonance phenomena and the related ultrafast electronic relaxation processes to determine charge transfer or electron delocalization times, such as the transfer of electrons from Fe^{3+} at the hematite NP interface into the surrounding aqueous solution.

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Abstracts of the Session - Science Highlights Part II

Wednesday, 11 December 2024 from 16:20 to 17:20

Bunsen-Hall at WISTA Event Center

Fragment libraries: How sociable are they, and can we do better?

Oliver Koch

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Fragment-based drug discovery has become an essential technique for developing small molecular probes or drugs.[1] Performing fragment screening with available fragment libraries is often tedious and time-consuming when selecting fragments for further extension, since the required growth vector direction is difficult or impossible to access synthetically. This synthetic tractability issue is widespread and commonly impeding fragment-to-lead projects.[2] St. Denis et al. termed these as non-sociable fragments that lack the needed growth vector for fragment extensions.[1] An analysis by us of 98 available fragment libraries with 561.762 unique fragments in combination with 6 Ultra-Large chemical spaces showed that on average 84% of each library is unsociable. Only 6% of the available fragments are highly sociable and follow-up compounds are easily accessible.

To alleviate the issue of intractable fragments, we designed a 96-membered highly diverse, and entirely sociable fragment library for crystallographic screening based on Enamine’s REALSpace [3]. For each fragment every growth vector can be elaborated with a multitude of different substituents. Hundreds to thousands of follow-up compounds modified at all growth vectors are available for each fragment from Enamine’s REAL Space. Additionally, tens to hundreds of thousands of larger and more complex leadlike molecules are accessible per library member, further expanded by scaffold-modified, alternative fragments. This allows for rapid exploration of the chemical space around a fragment of interest without much effort.

This fragment library has also yielded numerous hits in a recent crystallographic screening on mycobacterial thioredoxin reductase.

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Multimodal X-ray methods for dentistry: elemental diffusion out of fillings and into the tooth structure

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Dental materials used for tooth restoration often come into close contact with tooth materials, specifically dentine. This may lead to diffusion of elements through the tubules [1] and potential changes in chemical and structural properties. Dentine is a biocomposite, vital component of teeth composed of non-stochiometric carbonated hydroxyapatite (cHAP) nanocrystals and collagen fibers. It is traversed by micron-sized dentinal tubules extending from the pulp outward resulting in a high porosity of the material.

To understand chemical changes that may follow dental treatment, X-ray techniques can give valuable insights concerning the structure or density of the components as well as the elemental composition and chemical species of the elements. Within the DFG funded projects IXdent (Integrative X-ray techniques for chemical and structural characterizations of dental interzones) and InterDent (Material aging abutting restorations: predicting dentine sclerosis) we combine methodology at synchrotron radiation facilities such as BESSY II with spectrometers using laboratory X-ray sources for a sustainable use of resources.

Following controlled aging for months or years, we observe 3D elemental distributions by imaging of treated bovine tooth specimens. New insights are obtained through a combination of X-ray fluorescence techniques and X-ray absorption/transmission measurements [2]. The advantages of multimodal approaches will be discussed and insights into the nano-biocomposite dentine presented.

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Abstract of the Public Lecture

Wednesday, 11 December 2024 from 17:30 to 18:30

Bunsen-Hall at WISTA Event Center

Atmospheric Research in the Amazon: Photons, Aerosols, Clouds and a Flavor of Adventure

Christopher Pöhlker, Max Planck Institute for Chemistry, Mainz, Germany

The Amazon rain forest plays key roles in the carbon and water cycles, biodiversity, and the climate system. However, it has already been altered significantly by human activities, and more pervasive change is expected to occur.[1] Of particular concern is the interplay between deforestation, fire, and drought, which could lead to the loss of carbon storage, change precipitation patterns, and potentially trigger an irreversible transformation of the entire ecosystem.[2,3]

A fascinating facet of the research in the Amazon is the intense water cycle, where evapotranspiration, cloud formation and precipitation not only sustain the rainforest, but also influence regional and global climate patterns.[4,5] For clouds and precipitation to form, tiny airborne particles known as atmospheric aerosols are needed to condense water vapor into cloud droplets.[6] The concentration of these particles over the rain forest varies significantly, ranging from very clean, preindustrial-like conditions during the wet season to dense smoke pollution from widespread fires in the dry season.[7,8] How these strong changes in pollution alter clouds and, thus, the water cycle as the Achilles' heel of the ecosystem remains a critical yet unresolved question.

Here, I will take you on a tour into the Amazon rain forest, show you what our research at the Amazon Tall Tower Observatory (https://www.attoproject.org/) in the heart of the Amazon Basin is about and demonstrate how BESSY II helps us to literally shed light on some of the biggest open questions.

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Abstracts of the Young Scientists Session

Thursday, 12 December 2024 from 09:45 to 11:00

Bunsen-Hall at WISTA Event Center

Imaging Nanometer Scale Spin Textures and Their Picosecond Dynamics

Lisa-Marie Kern[1], V. Deinhart[2], M. Schneider[1], C. Klose[1], K. Gerlinger[1], R. Battistelli[2,3], D. Engel[1], C.M. Günther[4], F. Büttner[2,3], K. Höflich[5,2], S. Eisebitt[1,6], B. Pfau[1].

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The controlled manipulation of spins is central in spintronics research. Competing interactions in a magnetic material can lead to the emergence of complex nanoscale spin textures. Such texture can exhibit a single-particle character and a non-trivial topology. The magnetic skyrmion is the prototypical topological spin texture, possessing unity topological charge. Beyond skyrmions, there exists a zoo of topological spin textures which, so far, has remained largely unexplored in experiments. The drivers for manipulating nanoscale magnetic textures in our ferromagnetic multilayer systems are either spin-orbit torques (SOT), induced by electrical current pulses of a few nanoseconds, or ultrashort laser excitations of a few hundred femtoseconds duration. Direct imaging of the associated magnetization dynamics at the intrinsic nanometer length and nano- to picosecond timescales has proven challenging. Recently, the control of magnetic textures like skyrmions on the nanometer scale has been demonstrated [1]. Employing focused helium ion irradiation, we can artificially engineer anisotropy defects which serve as preferred sites for deterministic skyrmion nucleation in ferromagnetic thin films with perpendicular magnetic anisotropy (PMA). In addition, these tailored defects can act as origin and return point for the SOT- or laser-driven magnetization dynamics [2]. In this study, we demonstrate time-resolved x-ray imaging experiments to probe the response of the local magnetization during and shortly after an SOT or a laser pulse. Our images expose previously unseen chaotic magnetization dynamics, characterized by magnetic instabilities, and topological transformations. Moreover, we established a promising platform to study isolated topological textures under controlled conditions which may improve our general understanding of their emergence and intrinsic magnetization dynamics on picosecond timescales and with nanometer spatial resolution.

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Evidence of superconducting Fermi Arcs

Andrii Kuibarov[1], Oleksand Suvorov[1], Riccardo Vocaturo[1], Alexander Fedorov[1,2], Rui Lou[1,2], Luise Merkwitz[1], Vladimir Voroshnin[2], Jorge I. Facio[3], Klaus Koepernik[1], Alexander Yaresko[4], Grigory Shipunov[1], Saicharan Aswartham[1], Jeroen van den Brink[1], Bernd Büchner[1] and Sergey Borisenko[1]

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Numerous clever ideas have been proposed to generate Majorana fermions. As bulk topological superconductors remain elusive, the most promising approaches exploit proximity-induced superconductivity making systems fragile and difficult to realize. Materials with inherent topological properties, such as Weyl semimetals are also a potential candidate. Historically, the pursuit of Majorana fermions has focused on bulk superconductivity, overlooking the possibility of intrinsic superconductivity within Fermi surface arcs.

Here, by utilizing angle-resolved photoemission spectroscopy and ab initio calculations, we have identified topological Fermi arcs on two opposing surfaces of the non-centrosymmetric Weyl material, trigonal $PtBi_2$. We demonstrate that Fermi arc states on both surfaces become superconducting at temperatures around 10 K. Remarkably, the corresponding coherence peaks manifest as the strongest and sharpest excitations ever detected by photoemission from solids, underscoring their potential technological relevance. Our findings indicate that superconductivity in $PtBi_2$ can occur exclusively at the surface, rendering it a possible platform to host Majorana modes.

Accelerating the laser-induced phase transition in nanostructured FeRh via Plasmonic Absorption

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We use ultrafast x-ray diffraction (UXRD) to follow the dynamics of the laser-induced magneto structural phase transition in continuous and lateral nanostructured FeRh films with average size of ~0.5µm² [1]. In thermal equilibrium the first-order antiferromagnetic-to-ferromagnetic phase transition is accompanied by a gigantic lattice expansion ~0.6%. It proceeds after heating above ~370K via domain nucleation and growth, which is characterized by the co-existence of both phases throughout the transition.

In our time-resolved experiment we drive the transition using short optical laser pulses and use the high angular and temporal resolution of the KMC-3 XPP endstation in BESSY's low alpha operation mode to individually probe the structural Bragg peaks of either the ferro- or antiferromagnetic phases, respectively. Their integrals directly relate to the volume fractions of the respective phases [2] and thus our UXRD experiment yields the transient fraction of FeRh that has transformed into the ferromagnetic phase upon laser excitation.

In the continuous and inhomogeneously excited FeRh film, which is due to the limited penetration depth of the pump light in the metallic film, we find a two-step emergence of the ferromagnetic phase that is related to a fast rise in the directly laser-excited near-surface region and a subsequent growth of the ferromagnetic phase into the depth of the layer driven by heating the backside above the transition temperature via heat diffusion [3]. In addition, our results reveal that the ferromagnetic phase emerges on an 8ps timescale after direct photoexcitation but only on a 50ps timescale after the delayed heating above the transition temperature at the backside of the film via near-equilibrium heat diffusion.

In contrast, the ferromagnetic phase forms on the 8ps timescale in the nanostructured FeRh film. Here, even a weaker optical excitation can more efficiently drive the transition into the ferromagnetic of the nanoislands. Our calculation of the spatially resolved absorption taking the actual shape of the nanoislands into account, shows that a plasmonic absorption in the nanoislands leads to an enhanced and more homogeneous optical excitation, which preferably enables the fast pathway of the phase transition in the entire volume of the FeRh nanoislands and thereby drastically accelerates the laser-induced phase transition.

References

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Integrative structural biology to explore mitochondrial architecture

Evangelia Nathanail[1,2], Ashwin Karthick Natarajan[1], Edoardo Rolando[2], Max Ruwolt[2,3], Cecilia Clementi[2], Fan Liu[3], Oliver Daumke[1,2]

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Mitochondria possess characteristic membrane folds named cristae whose form and biophysical properties are controlled by the mitochondrial contact site and cristae organizing system (MICOS). Our group previously structurally characterized yeast orthologues of MICOS components Mic60 and Mic19 and the role of their assembly in cristae junction morphology, but structural information on the human MICOS complex remains elusive. We have solved the crystal structure of a helical bundle of hsMic60, found only in higher eukaryotes, to 2.78 Å and have characterized it as a possible oligomerization domain. Further studies on this undescribed domain shed light on the differences between fungal and higher eukaryotic MICOS and help us identify unique characteristics of its assembly. This serves as input for our effort to provide an integrative structural model of human MICOS, combining structural, biophysical and computational data, in order to learn how MICOS governs crista junctions and contributes to mitochondrial protein import.

References

Tobias Bock-Bierbaum, Kathrin Funck et al., Structural insights into crista junction formation by the Mic60-Mic19 complex. Sci. Adv. 8 (2022). DOI: 10.1126/sciadv.abo4946

Vortex dynamics in high temperature superconductors

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$YBa_2Cu_3O_{7-x}$ (YBCO)/ferromagnet heterostructures have great potential for a wide range of applications. Understanding of their properties is of upmost importance.

Using extensive measurements of the magnetic moment of the superconductor in close contact with a magnetic layer as a function of magnetic field, temperature and time, the impact of the magnetic layer on the superconducting properties of YBCO was investigated. It was shown that the presence of a magnetic layer strongly impacts the critical temperature, critical current density and the pinning landscape in YBCO [1,2].

In another type of experiment, in a YBCO thin film decorated with an YIG ($Y_3Fe_5O_{12}$) lamella it was possible to visualize bound and stable vortex-antivortex pairs [3]. We used a transmission soft X-ray microscopy technique. Results suggest that this characterization approach could be applied on various YBCO/magnetic heterostructures.

References

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Abstracts of the Session - Science Highlights Part III

Thursday, 12 December 2024 from 11:30 to 12:30

Bunsen-Hall at WISTA Event Center

Rashba-like Spin Textures in Graphene Promoted by Ferromagnet-Mediated Electronic Hybridization with a Heavy Metal

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Epitaxial graphene/ferromagnetic metal (Gr/FM) heterostructures deposited onto heavy metals have been proposed for spintronic devices due to their perpendicular magnetic anisotropy and significant Dzyaloshinskii–Moriya interaction (DMI), which enable both enhanced thermal stability and the stabilization of chiral spin textures. However, advancing toward this goal requires a fundamental understanding of the microscopic origin of these unusual properties. In this study, we elucidate the nature of the induced spin–orbit coupling (SOC) at the Gr/Co interfaces on Ir. In this work, using spin- and angle-resolved photoemission spectroscopy in combination with density functional theory, we demonstrate that the interaction between the heavy metals and the graphene (Gr) layer—via hybridization with the ferromagnetic metal (FM)—is the source of the strong spin–orbit coupling (SOC) in the Gr layer. Additionally, our studies of ultrathin cobalt (Co) films beneath Gr reveal an energy splitting of approximately 100 meV for in-plane spin-polarized Gr π-bands, while the splitting for out-of-plane spin-polarized bands is negligible. This is consistent with a Rashba spin–orbit coupling at the Gr/Co interface, which we identify as either the fingerprint or the origin of the Dzyaloshinskii–Moriya interaction (DMI). This mechanism disappears at larger Co thicknesses, where neither in-plane nor out-of-plane spin–orbit splitting is observed, suggesting that the Gr π-states become electronically decoupled from the heavy metal. These findings are crucial for the future applications of Gr-based heterostructures in spintronic devices.

Reference

B. Muñiz Cano et al., ACS Nano 2024, 18, 24, 15716–15728

Mechanism of mammalian egg coat hardening and slow block to polyspermy

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In addition to supporting the growth of the oocyte and protecting the developing embryo until it hatches, the mammalian egg coat or zona pellucida (ZP) carries out two essential functions at fertilization. First, it mediates the initial interaction between gametes; then, it permanently blocks polyspermy after the first egg-sperm fusion event.

Whereas there is significant variability in the molecules involved in the latter process, the basic egg coat architecture is highly conserved from mollusks to mammals, although with different requirements for gamete interaction in external and internal fertilizers. Our previous studies suggested how mollusk acrosomal protein lysin dissolves the egg coat non-enzymatically, following species-specific recognition of ZP-N domain repeats at the N-terminus of vitelline envelope receptor for lysin (VERL) – the primary sperm-binding subunit of the mollusk egg coat.

Interestingly, ZP-N domain repeats also constitute the N-terminal region (NTR) of ZP2, a major glycoprotein subunit of mammalian ZP filaments. Post-fertilization cleavage of the ZP2 NTR is vital for reproduction, as it creates an irreversible block to polyspermy, and ZP2 processing was proposed to regulate gamete interaction by inactivating a sperm-binding activity located upstream of the cleavage site. However, the specific molecular effects of ZP2 cleavage and their role in ZP hardening — a phenomenon that also takes place after fertilization — were not well understood. By combining X-ray crystallography, cryo-EM and biochemical approaches, we discovered that cleavage of the ZP2 NTR promotes its oligomerization. Furthermore, deletion of ZP-N1, the ZP-N domain preceding the cleavage site, alters the normal oligomerization dynamics of mouse ZP2 by enabling it to homodimerize without requiring processing. Mice homozygous for this altered ZP2 variant exhibit subfertility due to a semi-hardened ZP that allows sperm attachment but hinders penetration. Further structural analysis of native vertebrate egg coat material, together with AlphaFold-Multimer predictions of human ZP polymers, revealed that egg coat filaments consist of two types of protofilaments, type I (ZP3) and type II (ZP1/ZP2/ZP4). These intertwine into a left-handed double helix, with the NTRs of type II subunits extending outward.

Together, these findings suggest that the oligomerization of cleaved ZP2 creates cross-links within the ZP, thereby increasing rigidity and rendering it impenetrable to additional sperm. This mechanical block, being independent of the often rapidly evolving gamete recognition interfaces, represents a highly effective strategy for preventing polyspermy. At the same time, the absence of a lysin-like molecule raises intriguing questions about the specific mechanisms of egg coat-sperm interaction in mammals.

From a biomedical point of view, our structural information — in particular, the human ZP2 NTR data collected at BESSY — provides a crucial foundation for interpreting mutations in human *ZP* genes that are linked to infertility, as well as paving the way for developing targeted non-hormonal contraceptives.

References

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Understanding the electrocatalyst lanthanum nickelate by combining X-ray absorption spectroscopy and density functional theory

Marcel Risch[1], Achim Füngerlings[2], Marcus Wohlgemuth[3], Denis Antipin[1], Emma van der Minne[4], Ellen Marijn Kiens[4], Javier Villalobos[1], Felix Gunkel[3], Rossitza Pentcheva[2] & Christoph Baeumer[4]

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Electrochemical methods and X-ray absorption spectroscopy (XAS) are powerful tools to understand electrocatalysis on an atomistic level especially when combined with additional theoretical methods.[1] In one such efforts, we explore the effect of surface transformation on the water oxidation activity of $LaNiO_{3-\delta}$ electrocatalyst with (001), (110) and (111) surface orientation. We reveal that the overpotential of the (111) facet is ≈ 30 − 60 mV lower than for the other facets and found that its surface transformed into oxyhydroxide-like NiOO(H) as supported by differential XAS analysis (Fig. 1). Moreover, a structural mismatch of the transformed layer with the underlying perovskite for (001) and (110) influences the ratio of Ni^{2+} and Ni^{3+} to Ni^{4+} sites during the reaction and thereby the binding energy of reaction intermediates, resulting in the distinct catalytic activity of the transformed facet. [1] This insight into structural transformation and chemical processes on the studied facets, contribute to the knowledge-based design of materials as electrocatalysts, which are key to many applications in green chemistry.

[1] M. Risch, et al., Angewandte Chemie, 2022, **61**, e202211949, doi: 10.1002/anie.202211949Mater. 12, 836–841 (2013)
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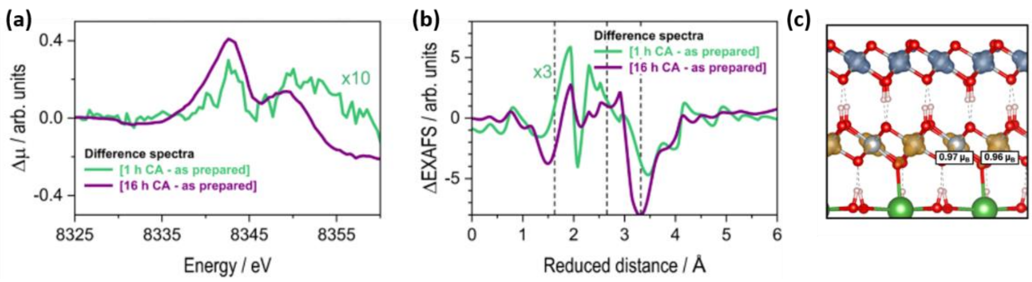

Figure 1. Differential (a) X-ray absorption near edge structure (XANES) and (b) extended X-ray absorption fine structure (EXAFS) of LaNiO3−δ samples treated mildly and harshly. (c) Surface structure of the transformed (111) facet from DFT+U showing stripes of low and intermediate spin Ni. Adapted from [2].

Abstracts of the Session - Science Highlights Part IV

Thursday, 12 December 2024 from 13:30 to 15:00

Bunsen-Hall at WISTA Event Center

Multimodal Investigations of Heterogeneous Interfaces

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The heterogeneous chemistry of solid-vapor, solid-liquid and liquid-vapor interfaces drives many important processes in fields as diverse as heterogeneous catalysis, electrochemistry, energy conversion, corrosion and atmospheric chemistry. These interfaces undergo complex chemical and structural changes under reaction conditions. Monitoring the evolution of the interfacial properties under as-close-to-realistic conditions as possible is the underpinning for the understanding of heterogeneous reactions on the molecular scale. A description of the physicochemical and morphological properties of complex interfaces requires the use of multiple complementary and interface-sensitive techniques to capture the details of, e.g., the chemical bonding of adsorbates, the charge state of the interface, and the reordering of the surface structure. In this presentation we will describe recent experiments that address some of these challenges and describe the concept of the future beamline for Enhanced Liquid Interface Spectroscopy and Analysis (ELISA) at BESSY II, which will enable simultaneous and collocal infrared and X-ray photoelectron spectroscopy as well as X-ray scattering experiments from the same sample location at liquid and solid interfaces.

Reference

S. Vadilonga et al., Synchrotron Radiation News **35**, 67 (2022).

Understanding the PhotoElectrochemistry of Diamond Water Interfaces

Arsène Chemin[1], Louis Godeffroy[1], Marin Rusu[1], Peter Knittel[2], Thomas Dittrich[1], Anke Krueger[3,4], Tristan Petit[1]

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Photoelectrochemistry utilizing renewable solar energy is expected to play a crucial role in the transition to a decarbonized society. With decreasing fabrication costs and scalable synthesis, synthetic boron-doped diamonds are emerging as ideal metal-free electrodes for electrochemical reactions in harsh conditions, such as water decontamination. These materials also act as a source of solvated electrons when exposed to UV light, enabling the chemical reduction of CO_2 and N_2 molecules [1-4]. Although the surface termination of diamond electrodes is known to be critical for photoactive processes, the intricate interplay between surface termination, photoactivity, and electrochemical reactions at solid-liquid interfaces remains poorly understood.

This study elucidates the role of surface states in diamond materials for charge separation and emission across deep UV to visible light excitation by correlating X-ray Absorption Spectroscopy with Surface Photovoltage Spectroscopy. Surface states are found to dominate sub-bandgap charge transfer [5]. In liquid environments, the effect of diamond surface termination on electron affinity, band bending, and charge extraction is investigated through photocurrent measurements in a photoelectrochemical cell. This reveals the synergistic effects of applied potential and light excitation in driving either surface redox reactions or solvated electron emission [6]. This work provides fundamentally new insights into (photo)redox processes on diamond materials, with potential applications in photoelectrochemical solar fuel generation and energy storage.

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In Situ P *K*-edge XANES Investigation of the Complex Aqueous H_3PO_3 Oxidation Behaviour

Romualdus Enggar Wibowo[1], Raul Garcia-Diez[1], Tomas Bystron[2], Marianne van der Merwe[1], Martin Prokop[2], Mauricio D. Arce[1,3], Anna Efimenko[1,4], Alexander Steigert[5], Milan Bernauer[2], Regan G. Wilks[1,4], Karel Bouzek[2], Marcus Bär[1,4,6,7]

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7 Dept. X-ray Spectroscopy at Interfaces of Thin Films, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), Germany.

Several studies suggest that H_3PO_4, a typical electrolyte in High-Temperature Polymer Electrolyte Membrane Fuel Cells (HT-PEMFCs), may undergo conversion to H_3PO_3 during operation [1,2]. This conversion poses potential challenges, as H_3PO_3 can poison Pt, the state-of-the-art catalyst of HT-PEMFCs, thereby reducing their performance [3,4]. Yet, a recent study also indicates that Pt might also catalyze the (re-)oxidation of aqueous H_3PO_3 back to H_3PO_4 [5]. This illustrates the complex interaction between Pt and H_3PO_x and highlights the need to understand the oxidation behaviour of H_3PO_3 under HT-PEMFC relevant conditions, necessary for optimizing the design of an efficient catalyst/electrolyte interface.

In situ P *K*-edge X-ray Absorption Near Edge Structure (XANES) spectroscopy was conducted to study the oxidation behaviour of aqueous H_3PO_3 under various conditions relevant to HT-PEMFCs operation. Experiments were conducted at the OÆSE end-station, at the two-color EMIL beamline at the BESSY II, HZB. Initial *in situ* XANES experiments coupled with electrochemical characterizations, indicate that intense irradiation induces the oxidation of H_3PO_3 through H_2O, resulting in the formation of H_3PO_4 and H_2. To minimize these undesirable irradiation effects, a broadly applicable experimental procedure was developed to minimize the local increase of irradiation dose, enabling accurate determination of the H_3PO_3 oxidation behaviour. Subsequently a series of *in situ* P *K*-edge XANES measurements were conducted under a varying range of experimental conditions: (i) temperature (25 vs 75°C), (ii) electrode roughness and Pt availability (‘Pt free’ Kapton, flat planar Pt, and rough Pt black), (iii) electrode potentials (open circuit potential vs more positive potentials [+0.8, +0.9, and +1.0 V_{RHE}]), and (iv) electrolyte concentrations (0.1, 1, and 5 mol dm^{-3}), thereby varying the H_2O content in the solution. The experiments with the different electrodes confirmed that Pt catalyzes the chemical oxidation of H_3PO_3 to H_3PO_4, which is enhanced by heat application, as confirmed by ex-situ ion exchange chromatography experiments. Additionally, electrochemical oxidation occurs upon the application of positive potentials. In fact, H_2O play a significant role in both chemical and electrochemical oxidation processes, as evidenced by the more pronounced oxidation of H_3PO_3 in electrolytes with higher H_2O concentration. These findings highlight the significant role of H_2O in the oxidation behaviour of H_3PO_3 and provide insights for potential adjustments in HT-PEMFCs operational conditions to mitigate Pt catalyst poisoning by H_3PO_3 [6].

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Enzymes for a sustainable plastic waste management

Parinita Singh[1], Da'san Jaradat[1], Zhishuai Li[2], Xu Han[2], Weidong Liu[2], Sabine Gavalda[3], Gregory Arnal[3], Vincent Tournier[3], Nicolas Chabot[3], Alain Marty[3], Ren Wei[4], Gottfried Palm[5], Uwe Bornscheuer[4], Manfred Weiss[1], Frank Lennartz[1] and Gert Weber[1]

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To counteract climate-change, the liberation of humanity from crude oil dependence is an urgent, ambitious and multi-faceted goal where biotechnology plays a key part. During the last 80 years, about 10 billion tons of synthetic polymers (plastics) have been synthesized and their ongoing crude-oil derived production still makes out most products (90%). Currently used (thermo-)mechanical or chemical recycling technologies typically have high energy costs and lead to a material downgrade in each round. In recent years, enzymes and microbes have become a viable option for sustainable biocatalytic re- and upcycling of plastics, paving the way towards circular economies. However, due to the complexity of different polymer types and their recalcitrance to biodegradation, these enzymes still must be improved before they qualify for industrial hydrolysis of synthetic polymers.

HZB has set out to biotechnologically improve plastic-degrading enzymes for hydrolysable polymer types like polyethylene terephthalate (PET), polyamides (PA), and polyurethanes (PU) on a structural basis. In recent years, PET has become the best characterized substrate for enzymatic hydrolysis. Starting with the structure-based enhancement of MHETase derived from the PET-degrading bacterium *I. sakaiensis*[1] we extended our research towards other PET hydrolases and characterized their substrate-binding modes[2]. Together with industrial collaborators, we suggest standardized protocols to help other studies reach large scale applicability[3]. Upon further improvement of the enzymes, we anticipate enzymatic PET hydrolysis to be a viable and competitive technology for future industrial recycling. Unlike PET, polyurethanes are difficult targets for enzymatic hydrolysis due to their material complexity and high additive content. With collaborators, we have structurally characterized the recently discovered polyurethanase (PUase) UMG-SP2, capable of hydrolyzing urethane bonds. Our work sheds first light on polyurethane hydrolysis and the respective enzyme function and paves the way towards the semi-rational improvement of SP2 and also other PUases.

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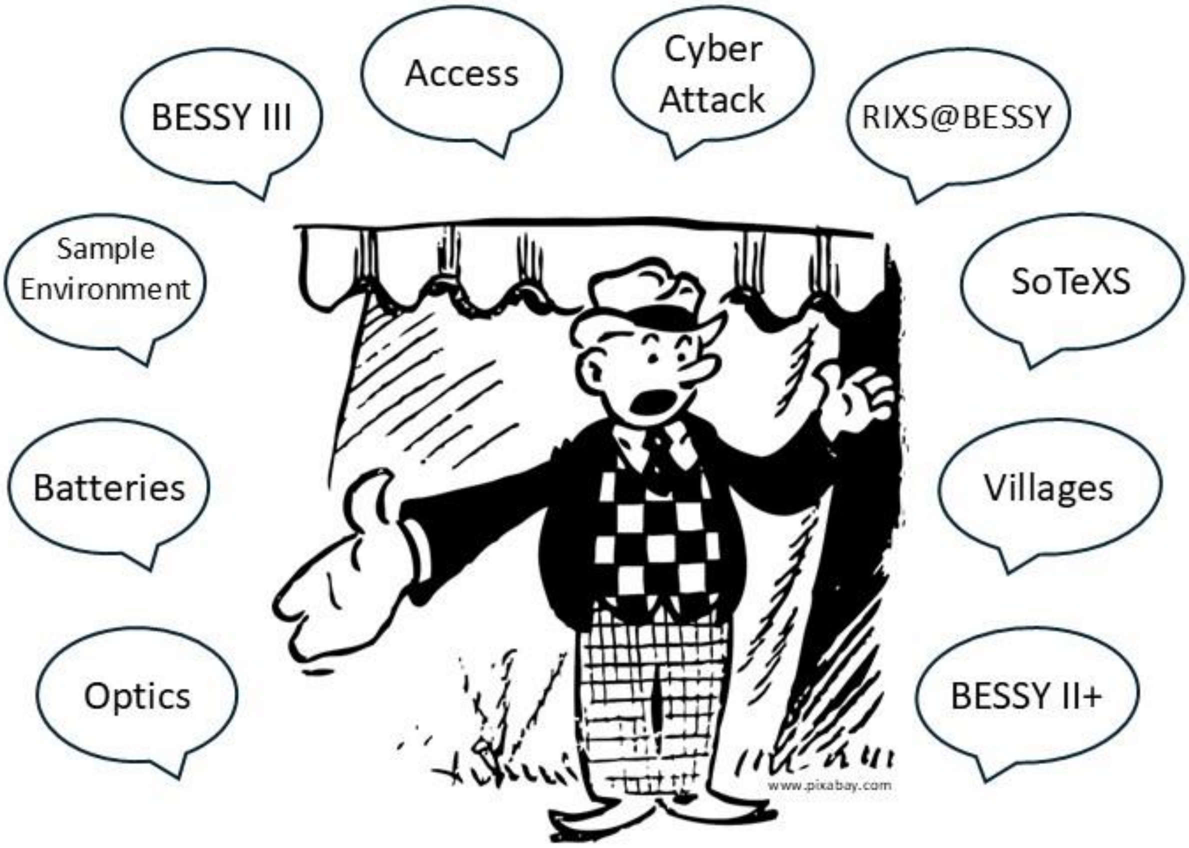
Please meet us at the

MARKETPLACE OF INNOVATIONS

for Discussion & Sweets

Thursday, December 12 from 15:30 to 17:00

BESSY II Lecture Hall



Abstracts of the Poster Session

Thursday, 12 December from 17:00 to 19:00

BESSY II Experimental Hall

39 Crystal structure of blue laccase BP76, a unique termite suicidal defense weapon

Jirí Brynda (Czech Academy of Sciences)

Aging workers of the termite Neocapritermes taracua can defend their colony by sacrificing themselves by body rupture, mixing the externally stored blue laccase BP76 with hydroquinones to produce a sticky liquid rich in toxic benzoquinones. Here, we describe the crystal structure of BP76 isolated from N. taracua in its native form.

40 Integrated Structure Biology Core Faacility at IOCB

Petr Pachl (Institute of Organic Chemistry and Biochemistry AS CR)

At IOCB in the structure biology group we are organising core facility that help members of other groups to reach specialized advices and equipment they need. We provide and maintain a crystallization room equipped with three crystallization robots, imagining system, several optical, and a UV microscope. On top of that we provide data collection at our home source and at synchrotron beam lines.

42 THE HZB-MX BIOLAB

Camilla Genter Dieguez (Helmholtz-Zentrum Berlin)

The HZB-MX BioLab supports the entire workflow of protein sample preparation, from gene to crystal. Our facility provides the necessary equipment and expertise for cell cultivation, protein expression, purification, characterization, and crystallization. The BioLab is operated by the MX-Group to support external and internal users in the preparation of their biological samples (safety level S1).

45 Structural insights into cancer-related enzyme CA IX

Adéla Fejfarová (Czech Academy of Sciences)

Proteins upregulated during cancer development represent attractive targets for anticancer therapy. In this structure-based drug design project we studied cancer-related enzyme carbonic anhydrase IX(CA IX) by macromolecular crystallography. The data collected at HZB MX-beamlines enabled us to determine protein structures by which we have gained insights into the CA IX complex formation on the cancer cells.

46 Engineering enzymes for biodegradation of synthetic plastic

Parinita Singh (Helmholtz-Zentrum Berlin)

Inadequate management of plastic waste has led to the accumulation of plastics in ecosystems and there is a need for effective plastic biodegradation, to promote bio-based circular economy. In this study, structural insights into the enzymatic hydrolysis of PET and TPU are given to scale up the enzymatic breakdown of plastics, especially for industrial-scale applications.

46 a Fragment screening against the SARS-CoV-2 macrodomain

Frank Lennartz (Helmholtz-Zentrum Berlin)

The macrodomain Mac1 from SARS-CoV-2 is an important pathogenicity factor during infection with coronaviruses, making it a promising target for drug development. Here, using X-ray crystallography, we have screened fragment libraries against Mac1, finding several hits that target its active site and are promising starting points for development into small molecule inhibitors against SARS-CoV-2.

47 From Uncertainty to Molecular Mechanism: Missense Mutations in BRAF and MAP2K1 in Cognitive Disorders

Petra Havlickova (University of South Bohemia)

The RAS/MAPK pathway regulates cell cycle and proliferation, and the mutations are driving cancer and developmental syndromes known as RASopathies, that lead to intellectual disability (ID) and autism (ASD). This study investigates de novo variants in BRAF and MAP2K1 found in ID/ASD patients. We analyze these variants' effects on kinase activity and structure to understand their role in disease.

48 Crystallographic compound screening as a tool towards new SARS-CoV-2 inhibitors

Laila Benz (Helmholtz-Zentrum Berlin)

The SARS-CoV-2 pandemic has had a significant global impact, with more than 775 million people infected and over 7.0 million deaths since it began. The main protease of SARS-CoV-2 (Mpro) is crucial for the viral life cycle and therefore a promising target. In this study crystallographic compound screening is used to find small molecule starting points to design high affinity binders against MPro.

49 Facilities for Macromolecular Crystallography at HZB

Uwe Müller (Helmholtz-Zentrum-Berlin)

This poster describes the current status and future directions of the MX facilities at HZB, including three macromolecular crystallography beam lines and associated facilities.

50 XDSAPP3 – the new graphical user interface for the convenient processing of diffraction data using XDS

Thomas Hauß (Helmholtz-Zentrum Berlin)

XDSAPP3 is a further development of the well-known program XDSAPP [1] to (semi-) automatically process diffraction data using XDS [2]. Improvements in decision making, the support for EIGER detectors, and additions to the GUI are some of the major advances. An outlook to the new XDSAPP version2 will be given. [1] Sparta, K. et al. (2016). J. Appl. Cryst. 49, 108 [2] Kabsch, W (2010) Acta Cryst. D66, 125-13.

51 The F2X Facility - Crystallographic Fragment Screening at HZB

Melanie Oelker (Helmholtz-Zentrum Berlin)

As part of the MX beamlines at HZB, the F2X facility supports user, who are interested in performing a crystallographic fragment screening with their target protein(s) as a crucial step in a drug discovery process. For this, the F2X facility provides required material and instruments as well as expert knowledge.

52 The Software Landscape of Macromolecular Crystallography Beamlines in the EU

David James (Helmholtz-Zentrum Berlin)

Synchrotrons across Europe have been collaborating for years to standardize their macromolecular crystallography software. Here we present the two principal actors: the MXCuBE stack which serves as the interface for crystallography experiments, and the ISPyB stack which serves as a backend repository for experimental metadata, as well as the architecture of their interaction.

53 Crystallographic fragment screening for StQNG1

Florian Flegler (Philipps-Universität Marburg)

In this work, a crystallographic fragment screening (CFS) was performed for StQNG1. StQNG1 is a model enzyme for QNG1 (queuosine nucleoside glycosylase 1) which is a potential drug target in cancer. From the fragment library composed of 98 compounds, 3 fragments were identified as binders. The ligand-bound structures were solved and the binding mode evaluated. This knowledge could be used as a starting point.

114 h Non-linear transient Coulomb screening of core excitons in wide band gap semiconductors

Thomas Rossi (Helmholtz-Zentrum Berlin)

We characterize the Coulomb screening induced by photoexcited carriers on core excitons in ZnO employing picosecond X-ray transient absorption, supported by state-of-the-art many-body computational methods. The Coulomb screening modification leads to a decrease in the core-exciton binding energy, which depends on both the excitation density and the distribution of photoexcited carriers in k-space.

114 k Investigation of Charge Dynamics in Lead Halide Perovskites at the PM4 LowDose Beamline

Alberto Garcia Fernandez (Uppsala University)

To further develop lead halide perovskites for solar cells, understanding their behavior under light is key. Using time-resolved photoelectron spectroscopy at PM4 beamline, we were able to study charge dynamics in $CsPbBr_3$ and $Cs_xFA_{1-x}PbI_3$ single crystals in different timescales (ps to ms and s to min).

115 Dynamics of Photovoltage Generation in Quantum Dot Solar Cells at PM4

Julia Prumbs (Uppsala University)

Quantum dot solar cells are an alternative to Si solar cells. Given the layered structure of these cells, studying charge transfer across interfaces is essential for understanding photon-to-electron conversion. Laser-induced pump-probe signals are measured using time-resolved XPS, reaching a time resolution of up to 100 ps at the LowDosePES endstation at PM4.

116 Using CoESCA to unlock complex electronic structures

Johansson Fredrik (Uppsala University)

Coincidence Electron Spectroscopy for Chemical Analysis (CoESCA) allows for separation of details in XPS spectra that are overlapping. The method using Auger- Photoelectron coincidences can reveal electronic interactions such as the formation of bonds between an adsorbate and a substrate as will be showcased with different examples.

117 COESCA station for coincidence electron spectroscopy on solids and surfaces: Progress and upgrades

Danilo Kühn (Helmholtz-Zentrum Berlin)

Synchrotron based angle-resolved time-of-flight electron spectroscopy enables highly efficient coincidence electron spectroscopy on solids and surfaces. Studies of the electronic structure of strongly correlated materials and surface layers will be discussed. Recent upgrades and a future prospect will be presented.

118 Soft X-rays for purely organic quantum materials

Arkaprava Das (Universität Tübingen)

We present our last results on purely organic radicals as potential candidates for spintronics and the opportunity for all users that our project, funded by the Federal Ministry of Education and Research (BMBF) offers. It allows us to implement a new experimental infrastructure at the CoESCA end station of the UE52 PGM beamline, making it available to the entire synchrotron user community.

119 Covalency in transition metal perovskite oxides $LaMO_3$ (M=Ti-Ni) and La_2CuO_4

Katarzyna Siewierska (Helmholtz-Zentrum Berlin)

In this work, we use resonant inelastic X-ray scattering (RIXS) at the lanthanum N4,5 edges and density functional theory (DFT) to investigate the hybridization mechanisms in $LaMO_3$. Our work evidences an observable contribution of localized lanthanum 5p and 4f orbitals in the band structure.

120 Platinum group metals by the light of XAS: spectroscopic insights on the heavy 5d transition metal oxides

João Pedro Massaria de Arcanto (Helmholtz-Zentrum Berlin)

The electronic structure of $[Os, Ir, Pt,O_x]^+$ in the gas-phase was studied using XAS at the IonTrap endstation (UE52-PGM). $[OsO_x]^+$, $[IrO_x]^+$, and $[PtO_x]^+$ (x=1-3) showed similar behaviour, being a true monoxido, dioxido and trioxido, OS of +3, +5 and +7, respectively. $[OsO_4]^+$ is an oxygen-centered radical, for $[IrO_4]^+$ two isomers are competitive, whereas $[PtO_4]^+$ is not completely elucidated.

121 First direct probing of the electronic structure of the oxygen-centered diradical $[ReO_4]^+$

Mayara da Silva Santos (Helmholtz-Zentrum Berlin)

Inorganic diradical species are scarce. Here, we confirm, via gas-phase X-ray absorption spectroscopy, the oxygen-centered diradical character of the tetraoxidorhenium(VII) cation. This adds spectroscopic characterization of the rhenium oxidation state and the nature of ligands to the known ability of $[ReO_4]^+$ to consecutively abstract two hydrogen atoms from methane. (DOI: 10.1002/cmtd.202400023).

122 Simulation of planar defects observed in synchrotron data

Götz Schuck (Helmholtz-Zentrum Berlin)

There is emerging evidence that planar faults play a significant role in the explanation of ordering phenomena observed in hybrid perovskites. This poster presentation will provide an overview of the phenomena observed in synchrotron data and of the methods that can be employed to simulate the observed diffraction phenomena.

123 Sulfido Chromate (II): Synthesis and Characterization of Structural, Electronic, and Magnetic Properties

Mohammadreza Ghazanfari (Freie Universität Berlin)

$K_2Cr_3S_4$, the first alkali metal sulfido chromate (II), was synthesized via solid-state methods and confirmed by X-ray spectroscopy. Cr ions show rare square planar and pyramidal geometries with distortions, exhibiting a magnetic moment of 3.60 µB. Quantum calculations reveal Jahn-Teller activity in this d4 system. Its optical and dielectric properties suggest potential in capacitors and insulators.

124 Mechanistic Insights into Flexible MOFs for Sensing, Logic Gate Construction, Gas Storage, and Separation Applications

Roztocki Kornel (Adam Mickiewicz University Pozna)

The spatiotemporal adaptivity of flexible metal-organic frameworks gives rise to novel phenomena that are not observed in their rigid counterparts. This not only broadens our knowledge of the universe of porous materials but is also important for technological advances. Herein, we will present a mechanistic understanding of the flexible platform UAM-1.

125 Tender synchrotron radiation for the development of photovoltaic absorber materials

Daniel M. Többens (Helmholtz-Zentrum Berlin)

The focus of BESSY II on soft X-rays, unique in Germany, provides opportunities for X-ray absorption spectroscopy and anomalous diffraction studies on chemical elements relevant for photovoltaic applications. At KMC-2, this has been employed to study temperature-driven phase transitions of halide perovskites by XRD and EXAFS. Quaternary and ternary chalcogenide semiconductors are studied using Anomalous X-rays.

126 Unique opportunities for element-specific magnetic studies in magnetic fields up to 30 T at UE46_PGM-1@BESSY II

Alevtina Smekhova (Helmholtz-Zentrum Berlin)

We advertise a new pulsed magnetic field setup enabling the performance of X-ray absorption spectroscopy and X-ray magnetic circular dichroism (XMCD) experiments under pulsed magnetic fields up to +/- 30 T with a duration of about 4.5 ms and at temperatures down to 8 K. Recent results obtained for high-entropy CrMnFeCoNi systems demonstrate new possibilities in conducting XMCD experiments.

128 Spintronic Oscillators Unveiled: Direct Imaging of Their Nanoscale Magnetization Dynamics

Steffen Wittrock (Helmholtz-Zentrum Berlin)

Spintronic nanooscillators are versatile components for communication, energy harvesting, and neuromorphic computing. This work presents direct imaging of their nanoscale magnetization dynamics, previously accessible only through simulations. Using advanced X-ray microscopy, we reveal complex, nonlinear phenomena, challenging existing theories, advancing device design, and enabling novel applications.

129 Probing magnetization dynamics with elemental resolution in epitaxial Fe/CoO bilayers and Co/Mn/Co trilayers

Jendrik Gördes (Freie Universität Berlin)

We study the ultrafast magnetization dynamics of an epitaxial Fe/CoO bilayer on Ag(001) and a Co/Mn/Co trilayer on Cu(001) in an element-resolved way by resonant soft-x-ray reflectivity. For the bilayer system, we observe a direct energy transfer from hot Fe electrons to CoO, while for the trilayer system, a difference in demagnetization time was measured depending on the Mn spin structure.

130 First experiments with ultrashort circular polarized soft X-ray pulses at FLASH 2

Niko Pontius (Helmholtz-Zentrum Berlin)

XAS and XMCD with circular polarized (cp) soft X-rays are powerful tools to probe magnetic dynamics. The Slicing Facility at BESSYII has been the first facility to offer cp X-ray. Only recently, FELs began to provide circular polarization. Since an upgrade of FLASH, an afterburner allows generation of cp X-rays up to 860eV. We present the first XMCD results at the L2,3 edges of Co, Fe and Ni.

131 Time resolved operando X-Ray absorption spectroscopy of chemical vapor deposition processes

David Mueller (Forschungszentrum Jülich)

The initial steps of the growth of TiO_2 by CVD were observed through in situ Ti-L-edge XAS, resolving an intermediate Ti species that could explain susceptibility of the growth mode to magnetic fields resulting in different polymorphs of the oxide. Multivariate numerical techniques, such as PCA, enabled quantification of species and elucidation of the complex growth kinetics.

132 Tuning of the ultrafast demagnetization by ultrashort spin polarized currents in multi-sublattice ferrimagnets

Deeksha Gupta (Helmholtz-Zentrum Berlin)

We will present the combined study based on the time-resolved X-ray magnetic circular dichroism (TR-XMCD) measured at the FEMTOSPEX endstation, BESSY II, and theoretical modelling based on atomistic spin-dynamics simulations, evidencing the spin-dependent hot electron (SPHE) induced demagnetization on the ultrafast time scale on FeGd alloy in a specifically designed spin valve structure.

133 Observation of distorted tilted conical phase at the surface of a bulk chiral magnet with resonant elastic x-ray scattering

Sina Mehboodi (Technische Universität München)

We observe a well-ordered surface state referred to here as a distorted tilted conical spiral (dTC) phase over a wide range of magnetic fields. The dTC shows characteristic higher harmonic magnetic satellites in the REXS reciprocal space maps. Skyrmions emerge following static magnetic field cycling and appear to coexist with the dTC phase at the surface of chiral magnetic insulator Cu_2OSeO_3.

134 Self-assembled monolayers of molecular spin-crossover (SCO) switches

Fabian Streller (Friedrich Alexander Universität Erlangen Nürnberg)

Spin-crossover (SCO) complexes are regarded as promising materials in applications such as spintronics, molecular electronics and ultra-high-density memory systems. Here we report a step by step formation of SCO-active single-layer films on Au(111) surfaces. The thus created specimens were characterized by x-ray photoelectron spectroscopy (XPS) and near edge x-ray absorption fine structure (NEXAFS).

135 Impact of Operation Relevant Conditions on the Chemical Structure of Pt in GaPt Alloys

Tzung-En Hsieh (Helmholtz-Zentrum Berlin)

The chemical and electronic structure of in-system prepared GaPt alloys are elucidated by lab-based and synchrotron photoelectron spectroscopy (PES) in EMIL. Our detailed investigation reveals the presence of multiple GaPt species at the alloy surface, which are differently affected by sample treatments mimicking the catalyst operations, i.e., alloy liquefaction, oxidation, and oxide removal.

136 The OAESE endstation in EMIL: operando X-ray absorption spectroscopy for energy materials

Raul Garcia-Diez (Helmholtz-Zentrum Berlin)

The new Operando Absorption and Emission Spectroscopy (OAESE) endstation in the Energy Materials In-situ Laboratory Berlin (EMIL) enables real-time study of energy materials under operational conditions by operando XAS, where the two-color EMIL beamline (80–10000 eV) supports complementary soft, tender, and hard XAS. We present the setup's modular design and the first scientific results.

137 Impact of Mn on the Chemical Structure Profile of Model Catalysts for Fischer-Tropsch Synthesis

Pinar Sakoglu (Helmholtz-Zentrum Berlin)

Fischer-Tropsch synthesis (FTS) offers an alternative pathway to produce sustainable fuels through the conversion of syngas (H_2+CO). Cobalt (Co) is a key metal, known for its high activity and C_{5+} selectivity. Manganese (Mn) as a promoter further enhances catalytic activity, especially when in the Mn^{2+} state. Co(0001) single crystals offers well defined surfaces to study Co-Mn interactions.

138 Operando Scanning Transmission X-ray Microscopy at MYSTIIC

Abbas Beheshti Askari (Helmholtz-Zentrum Berlin)

Recent upgrades at the scanning transmission x-ray microscope MYSTIIC have unlocked the ability to perform in-situ and operando experiments via specialized sample cells, enabling measurement in liquids as well as gases with temperatures up to 700 °C. The ability to observe chemical and morphological changes of materials during a chemical reaction are highly relevant in many fields of research.

139 Charge Storage Mechanism in V_2CT_X MXene for Aqueous Zinc-Ion Battery Studied by in situ X-Ray Absorption Spectroscopy

Andreas Weisser (Helmholtz-Zentrum Berlin)

V_2CT_X MXene has shown exciting performance in aqueous zinc ion batteries. We monitor the chemical bonding of V_2CT_X MXene electrodes during charge processes using in situ XAS at the V K- and L-edges. Changes in MXene surface chemistry during electrochemical cycling in 3M $ZnSO_4$ and 7M $ZnCl_2$ aqueous solution will be discussed considering intercalation of Zn ions versus redox reactions at the interfaces.

140 Spectroscopic investigation of sub-monolayer Pt thin films on MnO_x at EMIL

Manuela Arztmann (Helmholtz-Zentrum Berlin)

Herein the evolution of the metal-support interaction (MSI) of sub-monolayer Pt thin films on manganese oxide (MnO_x) were investigated by XPS and UPS at the Energy Materials In-Situ Laboratory Berlin (EMIL). Simplified model systems allow a controlled study of the MSI as a function of the metal thickness and its alteration at elevated temperatures, providing insights into the MSI of Pt catalysts.

141 Combining Electron and X-ray Microscopy for Operando Insights into the Evolution of Electrocatalysts Under Reaction Conditions

Chee See Wee (Fritz-Haber-Institut)

Electrocatalysts exist within a complex liquid environment and experience (electro)chemical driving forces that can change their structure and composition during reaction. Here, we show how a synergistic combination of transmission electron and X-ray microscopy using similar operando platforms can allow us to interrogate their restructuring and chemical changes under different applied conditions.

142 Wide-energy rapid-scan operando-XAS on energy materials at KMC-3

Michael Haumann (Freie Universität Berlin)

A versatile setup for operando X-ray absorption spectroscopy (XAS) at beamline KMC-3 provides facilities for in-beam electrochemistry and photoexcitation experiments. An energy range of ca. 2-18 keV is available. Rapid monochromator scans in a few seconds to minutes with energy resolving multi-element SD detectors provide superior signal quality. The focus is on energy materials and catalysts.

143 UNIFIT 2025 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

Ronald Hesse (Universität Leipzig)

Main focus of the advancement of UNIFIT 2025 was the optimization of the iteration procedure for the estimation of the transmission function T(E). The three methods of the T(E) estimation, i) Survey Spectra Approach (SSA), ii) Quantified Peak-Area Approach (QPA) and iii) Approach Transmission Function T(E), are clearly separated. The currently used method, the iteration error and calculation time are displayed.

144 Highly-Sensitive Ultraviolet Photoelectron Yield Spectroscopy: A versatile technique for materials analytics

Suresh Maniyarasu (Helmholtz-Zentrum Berlin)

UV based Photoelectron spectroscopy (PES), is a powerful technique to investigate the density of occupied states (DOS) of the energetically shallow states of metals, semiconductors, and their interfaces. Conventionally, the incident photon energy (Eph) is kept constant, mostly using He-I emission (hv = 21.2 eV, He-UPS), while the count rate of photoelectrons is measured as a function of their kinetic energy.

145 HMC Hub Matter

Mojeeb Rahman Sedeqi (Helmholtz-Zentrum Berlin)

The Helmholtz Metadata Collaboration (HMC) Hub Matter helps you to connect your data to the Helmholtz data ecosystem. We ensure that your data is FAIR (Findable, Accessible, Interoperable, Reusable) by providing guidance, training, quality metrics and benchmarking. Whether you are a PhD student, postdoc, technician, engineer or beamline scientist; we invite you to pass by and discuss how we can support you.

147 Towards site-specific chiral explorations in the attosecond regime

Markus Ilchen (Universität Hamburg / DESY)

We will present the initial milestones of chirality science at FELs in the gas phase, the status of advanced metrology schemes for variably polarized, high-power (X)FEL pulses at the attosecond frontier, latest results from our angular-streaking atto-campaign at the European XFEL, and the advent of related scientific prospects that are about to emerge at a variety of facilities worldwide.

148 Confocal micro X-ray fluorescence spectroscopy for interfacial analysis and depth profiling of NMC batteries in operando

Yannick Wagener (Technische Universität Berlin)

Li-ion batteries using NMC cathodes show ageing effects possibly due to transition metal (TM) dissolution. To investigate such processes in operando, depth resolved elemental analysis is needed. Confocal micro-X-ray fluorescence (CµXRF) spectroscopy both using lab and synchrotron instrumentation is a well-suited technique to visualize TM deposition on the solid electrolyte interphase in real time.

149 Following Iron from Spinach Leaves to Intestinal Cells: 2D µXRF Imaging of Iron Bio-/Fortified Spinach and Caco-2 Iron Bioavailability Testing

Bodhi Thümmler (Technische Universität Berlin)

Low absorption of food iron is the most common dietary micronutrient deficiency in the world. The BMBF-funded project EiBiG was launched to raise plant iron content & bioavailability. Iron bioavailability is studied via i.v. digestion/Caco-2 models. µXRF µXRF is used to analyze the spatial distribution of elements in iron bio-/fortified baby-leaf spinach, aiming to explore iron absorption mechanisms.

150 Heating cell for temperature-dependent NEXAFS spectroscopy on thin films

Jonas Kaiser (Technische Universität Berlin)

Near edge X-ray absorption fine structure (NEXAFS) spectroscopy is used to investigate the electronic structure of a sample. To study temperature induced changes, a novel cell is presented which facilitates the homogeneous heating of large thin film samples in vacuum. The performance is demonstrated with our laboratory NEXAFS system using a laser produced plasma source.

151 Tabletop transient NEXAFS spectroscopy on liquids with a laser-produced plasma source

Richard Gnewkow (Helmholtz-Zentrum Berlin)

Time-resolved soft X-ray spectroscopy with a tabletop laser-produced plasma source. The system enables the first static and transient experiments in the liquid phase to be performed in the laboratory for energies up to 1400 eV and with a time resolution of 500 ps.

152 Investigating zinc diffusion from dental restorations into dentine

Oleksandra Marushchenko (Helmholtz-Zentrum Berlin)

Dentine contains micron-sized tubules that may facilitate elemental diffusion from dental fillings into the tooth structure. Zinc, found in restorations, can alter the chemical composition of dentine. This study utilizes µ-XRF, nano- XRF, and SEM-EDX to investigate Zn diffusion in bovine dentine, leveraging each method's resolution and capabilities to explore from the micron to the nano scale.

153 XPS and NEXAFS spectroscopy for developement of the processes for synthesis of mesoporous and 2D carbon based materials and their functionalisation

Eva Kovacevic (Univeristé d'Orleans)

Carbonaceous mesoporous and 2D materials are very interesting as interface for composite materials, especially in the field of energy applications. Herein the focus is on development of low power plasma processes for their synthesis and treatment. Presented is ex-situ XPS and NEXAS study, with focus on the role of gas mixture, substrate type and temperature on the pore size and functionalization.

154 Molybenum disulfide catalysts for water electrolysis

Franziska Traeger (Westfälische Hochschule)

Molybdenum disulfide, MoS_2, has shown promising behaviour as a catalyst for the hydrogen evolution reaction (HER) in water electrolysers, i.e., for the production of green hydrogen. Its activity can be enhanced considerably by doping or by substitution of sulfur atoms. We present a combined photoelectron and neutron spectroscopic study of MoS_2 crystals as well as powders as such or doped with Co or N.

155 Oxidative Decarbonylation of an Azacalixpyridine Supported Mo(0)-Tricarbonyl to a Mo(VI)-Trioxo Complex with Dioxygen on Au(111) Surface

Thomas Strunskus (Universität Kiel)

The conversion of a Mo(0) tricarbonyl complex into a Mo(VI) trioxo complex supported by a tolylazacalix[3]pyridine ligand with molecular O_2 is investigated using a variety of spectroscopic and analytical methods. This reaction takes place in solution, in the solid state and as well in a molecular film adsorbed on noble metal surface Au(111) and can be accelerated by exposure to light.

156 HELIUM MANAGEMENT AT HZB

Bastian Klemke (Helmholtz-Zentrum Berlin)

Helium is a limited resource, which has seen a significant increase in price over the last years. Moreover, we saw several times a shortage of Helium on the global market that led to significant problems for the realization of planned experiments at our institute. For this purpose, we are developing hardware and software solutions for Helium Management, which enable us to monitor the Helium at HZB.

157 In-situ study of niobium oxide reduction process with XPS for superconducting RF cavity applications

Alena Prudnikava (Helmholtz-Zentrum Berlin)

To optimize vacuum heat treatment for SRF niobium cavities, surface chemical state data are essential. Using in-situ XPS, we examined the native oxide under UHV annealing, revealing impurity interactions that degrade cavity efficiency. Baking a single-cell 1.3 GHz cavity at 230°C/24 h doubled Q0 and preserved maximum field, enabling a patented local heating method.

158 Opportunities for quantum technology at European synchrotron radiation facilities

Anna Makarova (Helmholtz-Zentrum Berlin)

Here, we present our pilot project "Strategic access for quantum technologies" that aims to facilitate the use of the synchrotron and free-electron laser light sources by researchers from quantum technology. We provide an overview of the particularly suited methods and instrumentation as well as demonstrate examples where these have been successfully employed.

159 Electronic band structure of ferroelectrics

Marius Adrian Husanu (National Institute of Materials Physics)

Pb(Zr,Ti)O_3 (PZT) is the most common ferroelectric (FE) material widely used in solid-state technology. Despite intense studies of PZT over decades, its intrinsic band structure, electron energy depending on 3D momentum k, is still unknown. Here, Pb($Zr_{0.2}Ti_{0.8}$)O_3 using soft-X-rays is revealed.

160 On the induced effects of a nano-patterned anode on the performances of photovoltaic devices

Sorina Iftimie (University of Bucharest)

We evaluated how a nano-patterned anode, obtained by imprint lithography, affects the photovoltaic performances of an organic thin film-based device. The nano-imprinted pillars with heights and areas less than 100 nm and a pitch between them of 2 nm improved almost 10 times the short-circuit current and output power, compared with an identical flat sample. Keywords: imprint lithography, PV devices.

163 Investigating self-assembly of beta3 oligoamides under varying control strategies by Vibrational Sum Frequency Generation spectroscopy (VSFG) and Scanning Near-field Optical Microscopy (SNOM)

Zsuzsanna Heiner (Humboldt Universität zu Berlin)

Terminal-modified beta3 oligoamides create fibrous structures via hydrogen bond motifs, and their self-assembly is sensitive to environmental conditions. Different control strategies can manipulate their self-assembly. Here, we used label-free, surface-specific spectroscopy, VSFG, combined with the SNOM technique to investigate peptide fibrillogenesis under various controlled conditions.

162 IR study of the influence of metal-organic framework structures on the properties of proton-exchange membranes SPES

Ivan Gorban (Universidad Carlos III de Madrid)

Incorporating metal-organic frameworks into proton exchange membranes enhances their water uptake and conductivity. Thus, novel hybrid membranes based on copolymer of sulfonated PSU and PPSU, and MOF MIL-88a were developed. In-situ FTIR and micro-IR spectroscopy were used to investigate the dynamics of chemical bonds and the behaviour of guest molecules within these hybrid membranes.

165 Extreme ultraviolet optical constants for TiN, amorphous SiO_2 and SiN

Qais Saadeh (Physikalisch-Technische Bundesanstalt)

The determination of optical constants from titanium nitride, amorphous silicon dioxide and silicon nitride is presented in the Extreme Ultraviolet (EUV) range. From thin film samples, synchrotron reflectometry and Elastic Recoil Detection Analysis (ERDA) were used to collect photometric data and determine the stoichiometries, respectively. The determined optical data are compared with external literature.

166 About the last blank spots in the material data

Victor Soltwisch (Physikalisch-Technische Bundesanstalt)

We give an overview of PTB's work to close the last existing gaps in the field of optical constants. The task of determining consistent data across different beamlines from soft X-ray to EUV up to the VUV spectral range is an enormous metrological challenge. This work can only be realized through intensive cooperation with various partners such as HZB, imec, Zeiss and many others.

167 Multilayer-coated blazed grating for high transmission tender X-ray energy range monochromator

Andrey Sokolov (Helmholtz-Zentrum Berlin)

Multilayer-coated blazed and laminar gratings are very promising optics for high flux grating monochromators that can as well to cover the tender X-ray range which is difficult for commonly used single coated diffraction gratings or crystal monochromators. Several prototypes were fabricated and coated with different multilayers. A record efficiency up to 60% were achieved on several structures.

168 High-Resolution, High-Efficiency Spectrometers in the Soft X-ray Range

Jürgen Probst (NOB Nano Optics Berlin GmbH)

Reflection zone plates, an innovative class of 2D varied line space gratings, combine dispersion, two-dimensional focusing and reflection in one element, providing high efficiency at high energy resolution. Recent developments on fabrication on spherical substrates extend the range of high-resolution flat field spectra to +/- 50% around the design energy. J. Probst et al., Appl. Sci. 10, 7210 (2020).

169 Accessing Buried Interphases: Using Operando HAXPES to Connect Cell Performance with Chemical Decomposition in Anode-Free Solid State Lithium Metal Batteries

Zora Chalkley (Helmholtz-Zentrum Berlin)

In anode-free lithium metal (Li0) batteries, Li0 plated on a current collector degrades the electrode/electrolyte interface, forming products in the solid electrolyte interphase (SEI) that we probe with operando hard x-ray photoelectron spectroscopy. This analysis technique’s advantages are shown by the connection of cell behaviour to SEI composition in various solid electrolyte cells.

170 Probing ultrafast charge transfer dynamics in lead sulfide quantum dots using core-hole clock spectroscopy

Elin Cartwright (Uppsala University)

PbS quantum dots (QDs) are promising for photovoltaics due to their tuneable electronic properties and near-infrared absorption. Using Resonant Auger and Core-Hole Clock Spectroscopy at the Pb M-edge, we examine charge transfer in PbS QDs, bulk PbS, and PbI_2 references. Results show faster charge transfer in bulk and larger QDs, while smaller QDs and PbI_2 display slower rates due to quantum confinement.

172 The in-situ GIXS heuristic tool for efficient reduction of 2D grazing-incidence X-ray data

Reb Lennart (Helmholtz-Zentrum Berlin)

INSIGHT is a Python-based software tool for reducing and batch processing large grazing-incidence wide- and small-angle X-ray scattering data sets and extracting structural, orientational, and morphological information on thin films.

173 Solution-driven processing of calcium sulfate: the mechanism of the reversible transformation of gypsum to bassanite in brines

Tomasz Stawski (Bundesanstalt für Materialforschung und -prüfung)

We present a sustainable, low-temperature method for converting gypsum ($CaSO_4{\cdot}2H_2O$) to bassanite ($CaSO_4{\cdot}0.5H_2O$) using reusable high-salinity brines (NaCl > 4 M). In situ X-ray and Raman studies reveal enhanced bassanite stability in high-ionic-strength solutions, defying expected solubility predictions. This method enables controlled bassanite crystallization, aiding in efficient gypsum recycling.

174 Researching Automation of Gypsum Recycling

Tom William Ryll (Bundesanstalt für Materialforschung und -prüfung)

We present an automated system for in-situ analysis to optimize gypsum recycling, using a modular setup to investigate gypsum-to-bassanite conversion in brines at 90°C. Remotely controlled via PC, the system automates entire reactions. Real-time sampling through a glass capillary enables synchrotron XRD and Raman analysis. Data is processed via NMF and PCA, offering insights for sustainable recycling.

175 Kinetics of the mechanically induced ibuprofen-nicotinamide co-crystal formation by in-situ X-ray diffraction

Lucia Casali (Bundesanstalt für Materialforschung und -prüfung)

Mechanochemistry offers sustainable synthesis for pharmaceuticals, though scaling remains challenging. By combining time-resolved in situ X-ray diffraction with kinetic modelling on the mechanosynthesis of the co-crystal ibuprofen-nicotinamide, we identified the reaction-driving factors. This deeper insight opens the way for a scale-up of mechanochemistry in the pharmaceutical industry.

176 X-Ray Absorption Spectroscopy to Reveal the „Molecular“ Structure of Metal and Nitrogen doped Carbons Electrocatalysts

Simon Dietzmann (Bundesanstalt für Materialforschung und -prüfung)

High-performance electrocatalysts are required for energy conversion. Metal and nitrogen enriched carbons (M-N-Cs) are promising candidates as they are conductive and can be tuned to the desired properties by appropriate modification. Structural characterization is essential to understand and optimize the catalytically active sites at the pseudo-molecular level.

177 Synchrotron Imaging Techniques for the study of in-situ sintering techniques of LTCC systems

Mustapha Eddah (Bundesanstalt für Materialforschung und -Prüfung)

LTCC are ceramic/metal devices used for a wide array of applications. The radiographic and tomographic reconstruction of such devices is challenging due to the complex microstructure and presence of both strongly and weakly absorbing parts. This project aims to develop novel Synchrotron X-Ray imaging techniques to quantify structure and defect formation during sintering.

178 Exploring Local Structure during Mechanochemical Synthesis

Jacob Wilson (University of Birmingham)

Mechanochemistry uses mechanical force to induce chemical or physical changes in reagents. The technique introduces disorder and lattice distortions that lead to the formation of unique metastable phases. We are developing synchrotron-based techniques to analyse the local structure in situ during mechanochemical reaction, providing further insights into mechanochemical processes.

179 Synchrotron X-Ray Tomography Techniques at BAMline

Henning Markötter (Bundesanstalt für Materialforschung und -prüfung)

The BAMline at the synchrotron X-ray source BESSY II (Berlin, Germany) is supporting researchers especially in materials science. As a non-destructive characterization method, synchrotron X-ray imaging, especially tomography with hard X-Rays, plays an important role in structural 3D characterization. Examples of the imaging capabilities are shown, which allow for in-situ and operando experiments.

180 Multipurpose instrumentation for the monitoring of fluid dynamics in nanoporous solids by in situ time-resolved X-ray cryo-imaging

Volodymyr Bon (Technische Universität Dresden)

Porous solids are of paramount importance in developing new sustainable technologies, such as energy storage materials, advanced separation technologies and safety systems. Herein we present the instrumentation for time-resolved in situ synchrotron X-ray imaging at BAMline developed for characterization of porous solids by in situ radiography and tomography under gas loading.

181 Microstructural characterisation of aerospace ceramics via Synchrotron X-ray Computed Tomography

Paula Campos de Oliveira (Bundesanstalt für Materialforschung und -prüfung)

This study investigates the microstructural evolution of refractory ceramics applied in aerospace using Synchrotron X-ray Computed Tomography (SXCT). We analyse how processing and temperature affect factors such as agglomeration, microcracking, particle orientation, and pore interconnectivity. These findings offer insights for optimising the design of more sustainable aircraft engines.

182 Unlocking the Secrets of Battery Safety: A 4D X-ray Journey

Shahabeddin Dayani (Bundesanstalt für Materialforschung und -prüfung)

This study leverages high-resolution 4D X-ray imaging to investigate critical safety mechanisms in commercial lithium-ion batteries. By capturing real-time structural changes during subzero conditions and destructive events, this work reveals key insights into failure modes, paving the way for safer battery designs and improved performance.

183 Combining electron energy loss and X-ray absorption spectroscopies for quantitative analysis of heterogeneity in Ce-supported C_3N_4 catalysts.

Teodor Jianu (Max-Planck Institute for Colloids and Interfaces)

XANES, EXAFS, Electron Energy Loss Spectroscopy (EELS), and STEM imaging were employed in resolving and visualizing local atomic structures around Cerium atoms in Ce-supported Carbon Nitride (Ce-C_3N_4) single-atom catalysts. This work aims to discriminate and quantify minority Ce species (clusters and nanoparticles) formed alongside single atoms, thereby assisting optimized EXAFS data fitting.

184 Optimizing Parameters for XES Measurements

Cafer Tufan Cakir (Bundesanstalt für Materialforschung und -prüfung)

X-ray Emission Spectroscopy (XES) requires optimized experimental design for accurate emission line detection. This study integrates simulation-driven spectra predictions with a digital twin of the experimental setup to optimize parameters like geometry, crystal type, and alignment. This approach enhances spectral resolution, reduces uncertainties, and provides a framework for advancements in XES.

189 Synergistic Catalytic Sites in High-Entropy Metal Hydroxide Organic Framework for Oxygen Evolution Reaction

Arkendu Roy (Bundesanstalt für Materialforschung und -prüfung)

The integration of multiple elements in a high-entropy state is crucial in the design of high-performance, durable electrocatalysts. We have synthesized High-Entropy Metal Hydroxide Organic Frameworks (HE-MHOFs) under mild solvothermal conditions. This novel crystalline metal-organic framework (MOF) features a random, homogeneous distribution of cations within high-entropy hydroxide layers.

190 Low Temperature Tomographic In-Situ and Operando Studies in Energy Research

Nils Böttcher (Bundesanstalt für Materialforschung und -prüfung)

Lithium-Ion-Batteries (LIB) remain a key storage technology for the renewable energy transition. Regarding safety LIBs suffer from undergoing thermal runaway (TR). Detailed understanding of TR requires a combination of reliable abuse methods and non-invasive analytics. Synergies from BAM Cell Test Centre and BAMline Synchrotron X-ray CT enable now in-depth investigations of LIBs safety behaviour.

191 Rashba-like Spin Textures in Graphene Promoted by Ferromagnet-Mediated Electronic Hybridization with a Heavy Metal

Jaime Sánchez-Barriga (Helmholtz-Zentrum Berlin)

Through spin- and angle-resolved photoemission spectroscopy we demonstrate a tunable, large Rashba effect at graphene/ferromagnetic metal interfaces grown on heavy metals.

192 Characterization of a 2D Moire-Pattern in a Twisted $SrTiO_3$ Thin Film Transferred and Bonded to $SrTiO_3$ Substrate

Martin Schmidbauer (Leibniz-Institut für Kristallzüchtung)

We have used 2D grazing-incidence in-plane X-ray diffraction in order to investigate a twisted epitaxial $SrTiO_3$ thin film transferred and bonded on $SrTiO_3$ substrate. A highly periodic two-dimensional Moire pattern is formed at the film substrate interface, inducing a long-range order screw dislocation network.

193 Magnetic solitons in FeNiPdP thin plates as seen by resonant soft x-ray scattering

Victor Ukleev (Helmholtz-Zentrum Berlin)

We investigate the stabilization of magnetic skyrmions in a thin plate of noncentrosymmetric FeNiPdP crystal using small-angle X-ray scattering. We observed transitions between helical, soliton, and skyrmion phases under applied magnetic fields. Particularly, drastically different behaviours were observed for in-plane and out-of-plane field orientations.

194 PEAXIS: A Soft X-ray RIXS end-station for Energy and Quantum Materials

Deniz Wong (Helmholtz-Zentrum Berlin)

PEAXIS is dedicated to a variety of users in the field of quantum and energy materials. Among others, investigations on unique dispersive excitations in model quantum material systems were carried out. Furthermore, RIXS measurements were used to probe distinct chemical states of oxygen that contribute to the redox reaction inherent to next generation cathodes in rechargeable batteries.

195 Soft X-ray investigations of photoactive chromium complexes

Benjamin Van Kuiken (European XFEL)

The trivalent chromium molecules are ideal candidates for photoactive complexes from earth-abundant elements. We use soft X-ray spectroscopy to characterize the electronic structure and photophysics of Cr(III) coordination complexes. Cr 2p3d RIXS measurements have been performed at the PEAXIS instrument, and ps time-resolved L-edge XAS is performed was measured at UE52-SGM.

196 A new decomposition algorithm for in-situ X-ray absorption spectro-microscopy

Christoph Pratsch (Helmholtz-Zentrum Berlin)

X-ray absorption spectro-microscopy is a powerful tool for investigating the chemical composition of heterogeneous materials at the nanoscale. Here we present a new approach to reference-free data analysis using an iterative multi-parameter steepest gradient descent method that is significantly more robust in the presence of random fluctuations, making it a better choice for low-dose imaging.

197 Transmission soft and tender X-ray microscopy for nanoscale 3D imaging

Stephan Werner (Helmholtz-Zentrum Berlin)

The HZB operates a transmission X-ray microscope (TXM) for nanoscale soft and tender X-ray imaging at the U41-PGM1 undulator beamline at BESSY II. The advanced optical setup of the HZB-TXM permits spectromicroscopic as well as tomographic imaging of cryogenic samples. We will report on the unique imaging capabilities of the HZB-TXM and give an overview of recent results in material, energy and life science.

199 Deformation of chitin crystal by its protein matrix

Gargi Joshi (Technische Universität Dresden)

Pre-stressing, associated with the presence of minerals, is observed in biological materials as a strategy to resist deformation. C. salei spider tendon, a composite of chitin nanofibril embedded in a hydrated protein matrix is devoid of any minerals. We investigate its hydration mechanism using real-time SAXS/WAXS measurements and show that chitin crystal is pre-stressed solely due to its protein matrix.

200 Nonlinear Vibrational and Infrared Nanospectroscopy of a PAS-Domain Protein at Protein Interfaces

Montserrat Roman Quintero (Humboldt Universität zu Berlin)

PAS domains mediate protein interactions in signalling and localisation. This study investigates the interaction of photoactive yellow protein (PYP) with poly-L-lysine (PLL) using VSFG spectroscopy and MD simulations. We find PYP orients specifically at the PLL interface, driven by dipole-dipole interactions. IR-nanospectroscopy will further explore PYP's conformational changes under light activation.

200 a Advancing Photoemission Orbital Tomography Towards Absolute Electron Density Reconstruction

Hans Kirschner (Physikalisch-Technische Bundesanstalt)

Photoemission orbital tomography (POT) measures photoelectrons from molecular orbitals in momentum space, linking them to electron densities in position space via a plane wave approximation, though this can be inaccurate in 3D. We improve POT by adapting it for atomic and molecular orbitals, using neon and methane as benchmarks. This refinement yields more accurate reconstructions of electron densities.

200 b Ageing of hybrid halide perovskites precursor solutions: a SAXS study

Ana Palacios Saura (Helmholtz-Zentrum Berlin)

Despite the astonishing increase in efficiency of hybrid halide perovskite-based solar cells, their long term stability is still a challenge. We investigated the stability of $(MA,FA)Pb(I,Br)_3$ precursor solutions in different solvents (GBL, DMF, NMP, DMSO and mixtures thereof) using SAXS for 4 years and show that the agglomerates present in the precursor solutions remain stable over time.

200 c Traceable dimensional characterisation of DNA-origami nanostructures in solution by synchrotron-based small-angle X-ray scattering

Jerome Deumer (Physikalisch-Technische Bundesanstalt)

DNA origamis have various potential applications, so standardized characterization methods and reference materials are necessary to ensure the reliability and comparability of results. In this study, SAXS was performed on complex-shaped DNA origamis to characterize them, including uncertainties, with the aim of using them as reference materials for bio-based nanoparticles in life sciences and biotechnology.

200 d Ergebnisse eines internationalen Ringversuchs zur Untersuchung von Dünnschichtproben mittels Röntgenfluoreszenzanalyse

André Wählisch (Physikalisch-Technische Bundesanstalt)

Im Projekt „KALIB-RFA“ wurden verschiedene Dünnschichtproben entworfen, hergestellt und mit Methoden wie Röntgenfluoreszenzanalyse untersucht. Einzelelement-, Multielement- und Legierungsschichten mit Dicken von 10 nm bis 1000 nm sowie eine Batterieelektrode wurden in einem internationalen Ringversuch analysiert. Die Ergebnisse dienen als Grundlage für eine neue Technische Spezifikation.

CR 2 Time-resolved X-PEEM imaging: vibrational modes and magnetic domains in 2D materials

Alevtina Smekhova (Helmholtz-Zentrum Berlin)

Here, we combine the X-PEEM imaging with an opportunity to perform time-resolved experiments for studies atomically thin heterostructures based on the van der Waals Fe_xGeTe_2 ferromagnet covered with the h-BN layer. The magnetic domains found in the Fe_xGeTe_2 layer at 40 K and vibrational modes found for pure h-BN demonstrate their time evolution on the ns scale after the fs laser excitation.

CR 4 The effects of ultrahigh vacuum treatments on SnSe flakes transferred on naturally oxidized Si wafers

Amelia Bocirnea (National Institute of Materials Physics)

The as introduced samples, as well as the treated flakes were fully characterized at the SMART beamline. The flakes did not show surface crystallinity; however the structures are 2D since a mild, 1 minute Ar^+ sputtering treatment considerably reduced the thickness of the structures. The flakes are highly affected by annealing and new interface phenomena occur during the solid state reaction at 350C in UHV.

CR a Hybrid metrology: CD-SAXS and GEXRF for nanostructure characterization

Analía F. Herrero (Physikalisch-Technische Bundesanstalt)

The properties of nanostructured surfaces are determined by their composition, size and shape. To characterize complex 3D nanostructures we propose the simultaneous use of two methods: critical-dimension small-angle X-ray scattering (CD-SAXS) with grazing-exit X-ray fluorescence (GEXRF), in a so-called hybrid method. Here, we report on the first steps in the combination of these methods.

CR b On the way to one push button synchrotron measurements

Michael Kolbe (Physikalisch-Technische Bundesanstalt)

To efficiently utilize measuring time, PTB is working on automating standard measurements. A one-push button operation based on PTB's measurement program has already been implemented in some experiments and is working stable. Here, we will share some insights into our implementation.

CR c PTB’s new microfocus beamline for Tender X-rays at BESSY II

Matthias Müller (Physikalisch-Technische Bundesanstalt)

We have set up a new beamline on a dipole which provides monochromatized radiation from 1.5 keV to 10 keV and a focused beam spot of typically 20 µm x 20 µm. The beamline combines two monochromator modules, a double crystal monochromator (DCM) with two Si 111 crystals and a plane grating monochromator (PGM) with a multilayer-coated blazed grating and plane mirror. A KB optic with two plane-elliptical mirrors.

CR d Large solid angle detector calibration for nano-XRF in the soft energy range

Leona Bauer (Technische Universität Berlin)

STXM in the soft X-ray range, equipped with an energy-dispersive detector (STXM-XRF), facilitates the measurement of elemental distributions in the nanometer range. Energy-dispersive SDD detectors with a large solid angle of detection increase the detection efficiency compared to conventional SDD detectors. We will present the detector calibration procedure and the first results of validation measurements.

CR e Quantitative X-ray photon beam damage investigations of solid-state electrolytes for LiS batteries

Lena K. Mathies (Physikalisch-Technische Bundesanstalt)

Quantitative radiation damage studies of solid electrolyte materials for LiS batteries were performed. Reference-free X-ray Fluorescence gives access to absolute elemental mass depositions and chemical speciation of elements. NEXAFS is applied to monitor dose dependent radiation induced changes. With absolute radiometrically calibrated instrumentation radiation damage thresholds are determined.

PTB 1 X-ray spectrometry study of Organo-Sulfur Batteries

Hongfei Yang (Physikalisch-Technische Bundesanstalt)

In this study, the X-ray absorption spectroscopy are utilized to characterize the organo-sulfur batteries as they provide valuable insight into the electronic structure and speciation of sulfur within complex chemical environments. We intent to quantify the sulfur strand lengths by identify the characteristic spectra feature, and expect it to be a critical parameter for battery stability.

PTB 2 Investigating EUV degradation with in-situ EUV transmission measurements

Duncan Ramsamoedj (University of Twente)

Material degradation in EUV is not yet fully understood due to the dependence on its electronic structure. We investigate the degradation of transition metal (TM) oxide (TMO) cap layers during EUV exposure. We hypothesize oxygen release from a TMO due to Auger decay, oxidizing the underlayer (SiNx), if a TM atom has no free valence electrons (VE). Inversely a TM atom with free VE is stable in EUV.

PTB 3 Reflectance measurements on silicon pore optics for the NewAthena observatory

Michael Krumrey (Physikalisch-Technische Bundesanstalt)

NewAthena will be the largest X-ray observatory ever flown. To achieve an effective area of 1 m² at 1 keV, a total polished mirror surface of 300 m² is required due to the grazing incidence. Based on silicon pore optics (SPO), a large X-ray lens with a diameter of 2.5 m will be composed of about 500 mirror modules (MM). The MMs are assembled and tested in the PTB laboratory at BESSY II.

PTB 4 Self-absorption correction of NEXAFS spectra for intermediate sample thicknesses applied to organo-sulfur model compounds

Konstantin Skudler (Physikalisch-Technische Bundesanstalt)

NEXAFS spectra measured in fluorescence-yield mode get damped due to self-absorption effects in samples which are neither thin nor dilute. Compared to established methods, the presented novel forward self-absorption correction is widely applicable, especially for intermediately thick and concentrated samples. The forward correction is applied to organo-sulfur liquid films as a proof of concept.

PTB 5 Time-resolved interface characterisation in Na-ion and lithium-sulphur batteries using quantitative X-ray absorption spectroscopy in the soft X-ray range.

Katja Frenzel (Physikalisch-Technische Bundesanstalt)

Next-generation batteries present sustainable alternatives to Li-ion batteries for grid stabilization. Achieving enhanced efficiency and longevity demands in-depth analysis of interface formation processes. Reference-free X-ray fluorescence combined with X-ray absorption spectroscopy enables quantitative operando insights, as shown in studies of Na-Ion SEI formation and LiS cathode CEI degradation.

PTB 6 Investigation of electronic structures using a new wavelength-dispersive spectrometer for advanced X-ray analysis

Moritz Winkler (Physikalisch-Technische Bundesanstalt)

Resonant Inelastic X-ray Scattering probes the electronic structure of matter. The new wavelength dispersive dual arm RIXS spectrometer located at the PGM Beamline was recently commissioned. Current applications are the investigation of energy materials, the determination of x-ray fundamental parameters and as support of quantum chemical calculations development.

PTB 7 Metrological Characterization of Nanoparticles by Small-Angle X-ray Scattering for Innovative Healthcare Applications

Robin Schürmann (Physikalisch-Technische Bundesanstalt)

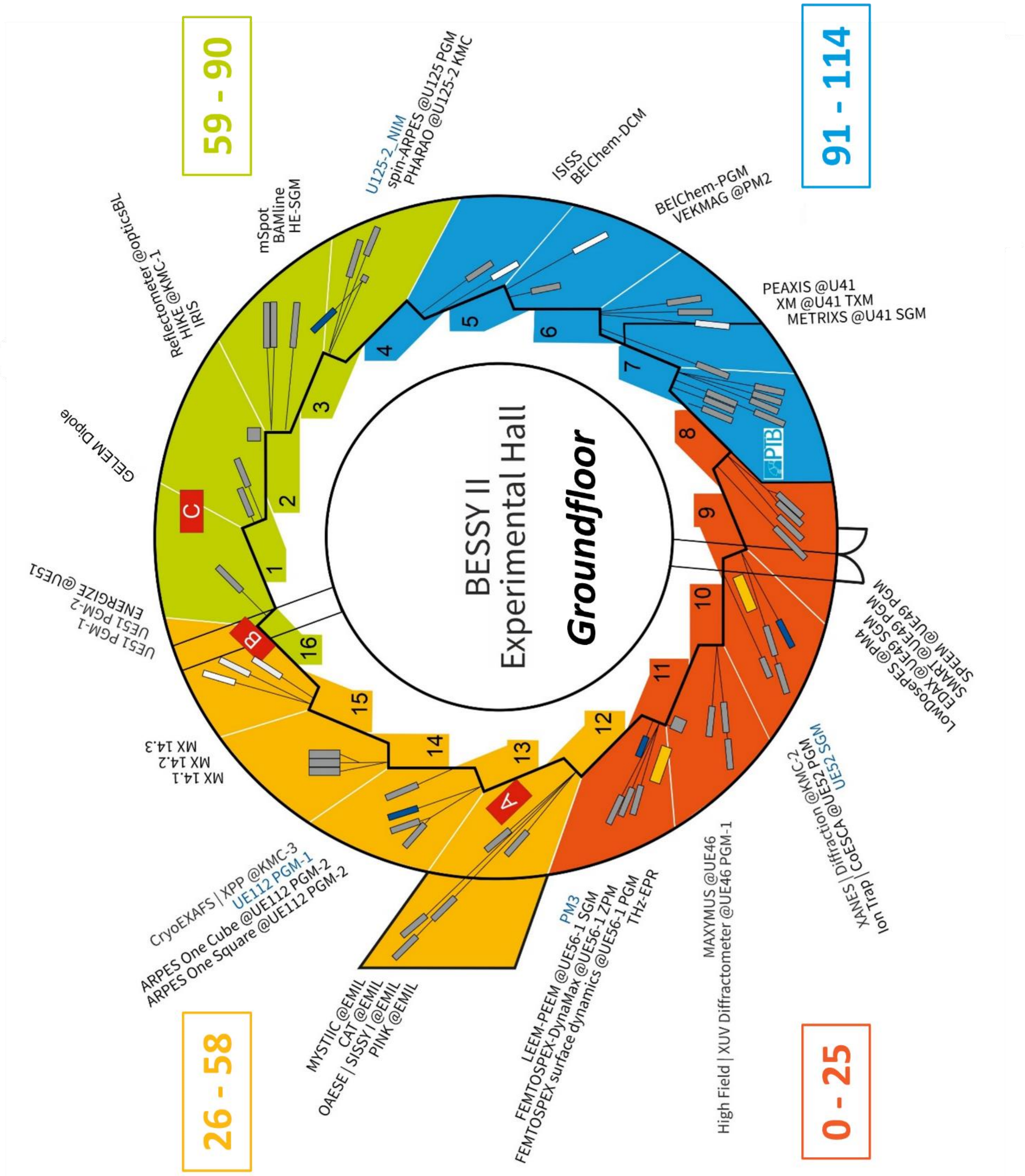
Small-angle X-ray Scattering (SAXS) can measure the size, shape, internal structure and number concentration of nanoparticles. Traceable SAXS measurements are critical for the development of reference materials, which are urgently needed to calibrate instruments in bioanalytical applications and to ensure accuracy and reliability in the assessment of critical quality attributes of nanotherapeutics.

PTB 8 Optical Characterization of Amorphous Silicon and Silicon Dioxide Thin Films from EUV to VUV Spectral Ranges

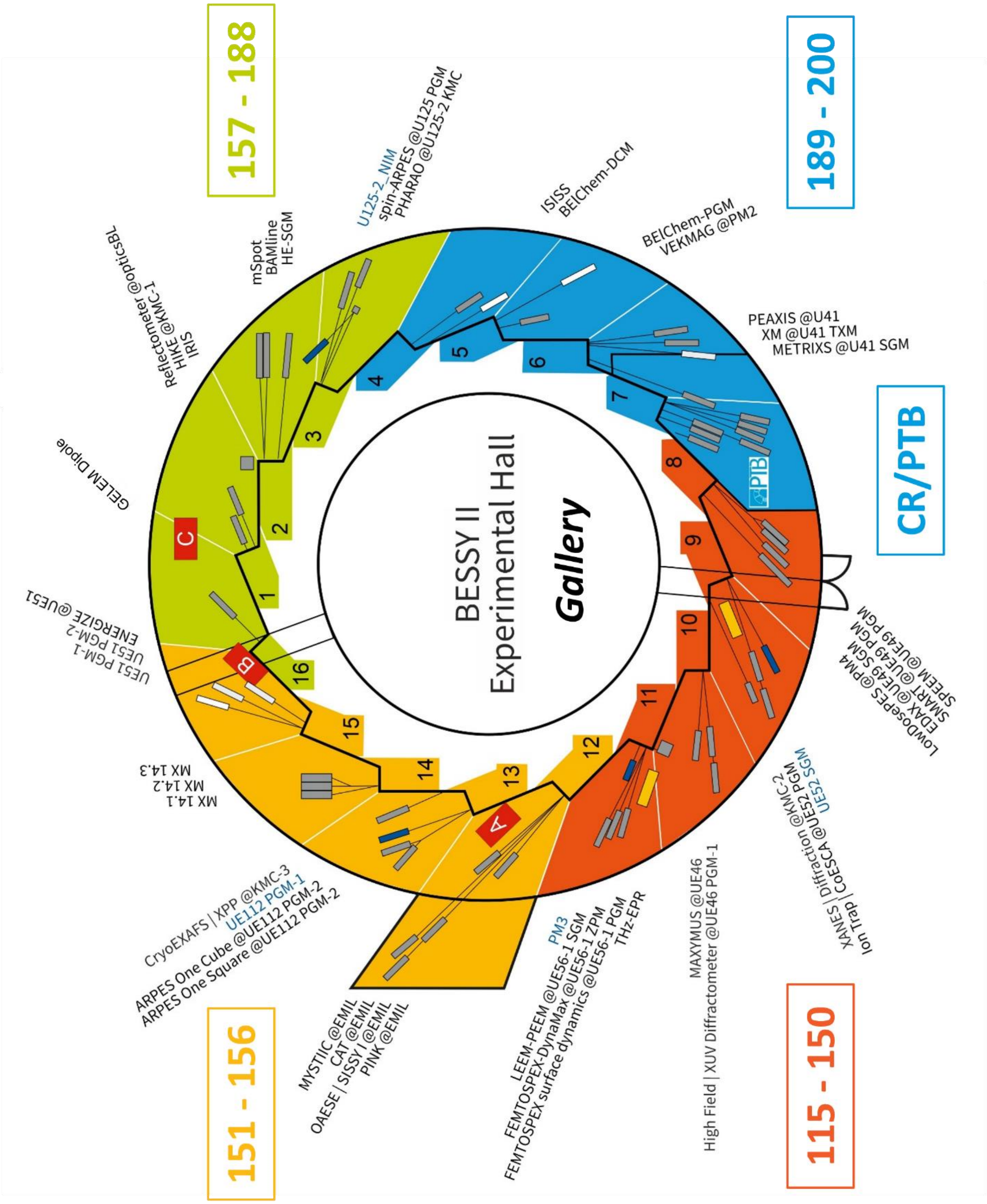
Abbasirad Najmeh (Physikalisch-Technische Bundesanstalt)

This study explores the optical properties of amorphous silicon and silicon dioxide thin films by determining their optical constants from EUV to VUV spectral ranges using reflectometry. The findings are crucial for improving the design and performance of semiconductor components, such as photomasks and optical coatings, which are essential in high-resolution lithography and inspection systems.

Floor Plan Poster Session - Groundfloor



Floor Plan Poster Session - Gallery / First Floor



Procedure 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 HZB User Committee is

29. November 2024 [00:01 CET] - 12. December 2024 [23:59 CET]

Eligible users are defined as users of HZB facilities, who have been actively registered in 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 via email by the election committee. In order to be able to vote, the users must be registered in GATE.

The candidates for the legislative term 2025/26 are

Volodymyr Bon	Technische Universität Dresden, Germany
Franziska Emmerling	Bundesanstalt für Materialforschung und -prüfung, Germany
Michael Weyand	Universität Bayreuth, Germany
Justin Wells	University of Oslo, Norway

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

Christian Gollwitzer	PTB	Representative of HZB User Committee
Olaf Schwarzkopf	HZB	Representative of HZB Director's Office
Beatrix-Kamelia Menzel	HZB	Representative of HZB User Coordination

Please find more detailed information on your HZB User Committee at:

https://www.helmholtz-berlin.de/user/general-information/user-committee/index_en.html

Friends of Helmholtz-Zentrum Berlin e.V.

The purpose of the Association of Friends of Helmholtz-Zentrum Berlin e.V. 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 Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) in Berlin or Deutsches Elektronen-Synchrotron (DESY) in 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, IBAN: DE48 1007 0000 0414 4440 00, BIC: DEUTDEBBXXX). 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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Hiermit beantrage ich die Aufnahme in den Verein Freundeskreis Helmholtz-Zentrum Berlin e.V.

Herewith I apply for admission to the Association Friends of Helmholtz-Zentrum Berlin e.V.

Angaben zur Person/personal data		
Anrede/salutation	Nachname/last name	Vorname/first name
Geburtsdatum/date of birth	Staatsangehörigkeit/nationality	
Titel/title	Berufsbezeichnung/profession	
Institution/institution		
Name/name		
Abteilung/department		
Straße/street		
PLZ/zip Ort/city/district		
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Homepage of institution		

Die jährlichen Mitgliedsbeiträge betragen derzeit für natürliche Personen EUR 40,-, für juristische Personen 150,- Euro, 100,- Euro oder 50,- Euro, für Studenten 10,- Euro.

The regular annual membership fees amount to 40,- Euro for natural persons, 150,-/100,-/50,- Euro for legal entities, 10,- Euro for students.

Art der Person/character of person: natural person _____ legal entity _____

Mitgliedsbeitrag/membership fee: _________ Euro

Im Rahmen freiwilliger Höherstufung/voluntary upgrading: _________ Euro

Datum/date: Unterschrift/signature:

Vendor Exhibition

Wednesday, 11 December from 10:00 to 16:30

Thursday, 12 December from 09:00 to 15:00

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Floor Plan - Vendor Exhibition at WISTA Event Center

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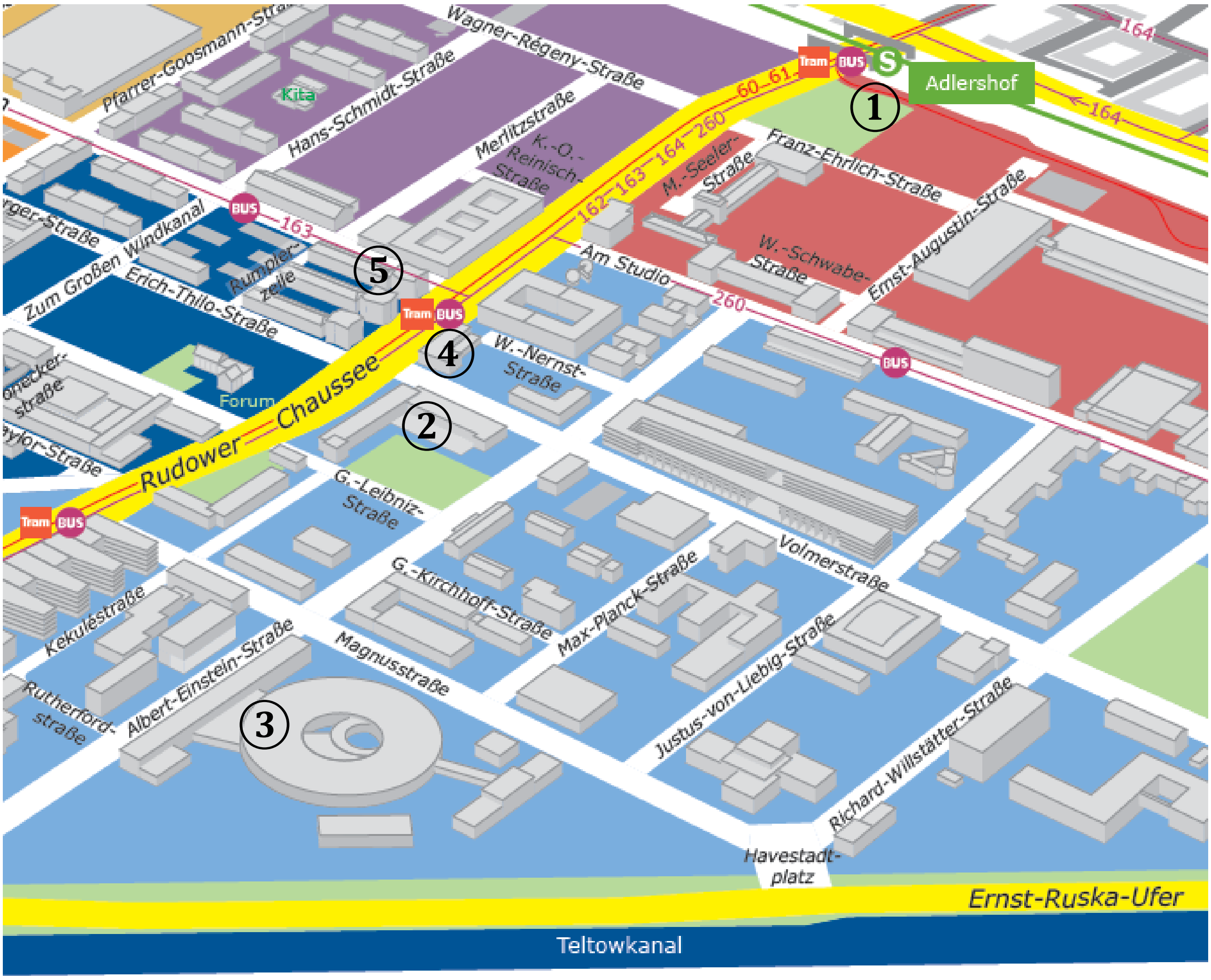
Campus Map Berlin-Adlershof

Helmholtz-Zentrum Berlin
Albert-Einstein-Straße 15
12489 Berlin

WISTA Event Center
Rudower Chaussee 17
12498 Berlin



① Train station Adlershof

② WISTA Event Center
Registration
Bunsen-Hall
Vendor Exhibition

③ BESSY II
Poster Session
Marketplace of Innovations

④ Hotel Essential by Dorint

⑤ Airporthotel Adlershof

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CALL FOR BESSY II PROPOSALS

Next allocation period: July 2025 to January 2026

Please submit your BESSY II beamtime proposal via the general access tool GATE (http://hz-b.de/gate)

DEADLINE
1 March 2025