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HZB BESSY II Light Source

15th BESSY@HZB USER MEETING

22 - 23 June 2023

BESSY II & WISTA Conference Center in Berlin-Adlershof

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Welcome

Dear Users and Friends,

Welcome to the 15TH BESSY@HZB User Meeting 2023.

This year's meeting is a very special one. It is the first live and on-site meeting after the three-year break caused by the Corona Pandemic. This is the first user meeting in summer and also the premiere of a new feature: the "Country of Honour". From now on – in order to make international integration and cooperation more visible - each BESSY@HZB User Meeting will feature a country of honour. This year's country of honour is Kenya and we are very pleased to welcome 17 Kenyan scientists as well as students from six Kenyan Universities who will participate in a twinning programme and in the user meeting.

This year's Public Lecture, a Public Panel Discussion on "Science Diplomacy, International Collaboration and the Contribution of Synchrotrons to Cooperative Solutions" takes up the new "Country of Honour" feature and will certainly be the highlight of the programme. We are very delighted to present the following highly regarded panel list: Prof. Dr. Rolf-Dieter Heuer (former General Director of CERN), Prof. Dr. Sekazi K. Mtingwa (*LAAAMP* Executive Committee), Dr. Gihan Kamel (SESAME), Dr. Lucy Ombaka (Technical University of Kenya), and Dr. Yazmin Lucero Cobos Becerra (HZB).

This year's user meeting is also a great opportunity to celebrate the 25th anniversary of BESSY II. In September 1998 BESSY II in Berlin-Adlershof offered the first user beam. For decades, science in Berlin has been an important driver of innovation and progress. Many discoveries - from fundamental insights to marketable products - are the result of research with synchrotron light. Despite regular upgrades, we will reach the limits of modernisation in the foreseeable future. We are facing new challenges and our user communities as well as their demands are subjects to constant change. To be prepared for the prospective challenges HZB has developed the BESSY II+ upgrade programme of the facility BESSY II with the three major goals: (1) creating new experimental possibilities, especially for operando investigations: The aim here is to investigate samples – such as batteries or solar cells - "at work", (2) modernising the accelerator, upgrading the technical infrastructure, and expanding digitalisation and automation and (3) developing further the research facility in terms of sustainability - from photovoltaics on the roof to sustainable research data ("FAIR data"). BESSY II+ will help us to bridge the "research gap" before the new BESSY III synchrotron is scheduled to go into operation in the mid-2030s. You are invited to learn more about our latest developments in our synchrotron session on Thursday morning.

We have again compiled a very interesting and diverse programme. You can join us on a journey of Jordan's history and dive deep into the world of marine ecosystems. You will learn about cadmium in chocolate and how plants deal with the day-night cycle. The latest results on catalysis and battery materials will cover the field of energy research and you will be excited to be informed about recent developments on information technology and photon science. Once again, the Ernst-Eckhard-Koch Prize for an outstanding doctoral thesis and the innovation Award on Synchrotron Radiation bestowed by the "Freundeskreis Helmholtz-Zentrum Berlin e.V." bears witness to the outstanding research performed by our users and colleagues.

The social highlight of this years' summer meeting will certainly be the outdoor party on Friday evening. This has been kindly sponsored by companies taking part in the industrial exhibition and is celebrating the BESSY II's 25th anniversary.

Two satellite workshops "Minerva-Gentner-Symposium: Bringing the sea to BESSY" and "Probing functionality with soft x-rays" complete the meeting.

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

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

Sincerely,

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

Programme Day 1 / 22 June 2023 / Thursday		
09:00 - 17:00	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 - 10:10	Bernd Rech (HZB) - Welcome to the User Meeting 2023	
10:10 - 10:30	Antje Vollmer (HZB) - News from BESSY II and BESSY III	
10:30 - 10:50	Markus Ries (HZB) - Operation and Development of BESSY II and MLS	
10:50 - 11:05	Frank Siewert (HZB) - On recent developments in Optics for science in the soft- and tender-X-ray energy range at BESSY-II and BESSY-III	
11:05 - 11:20	Gregor Hartmann (HZB) - Machine learning applications for the experimental environment	
11:20 - 11:35	Annette Pietzsch (HZB) - Probing functionality with soft x-rays	
11:35 - 11:50	Eugen Weschke (HZB) - Soft X-Ray spectroscopy and scattering at 30 Tesla: A new pulsed field setup at UE46	
11:50 - 12:00	The European Synchrotron and FEL User Organisation (ESUO)	
12:00 - 13:00	Lunch Break	Canteens on-site
13:00 - 14:50	**Science Highlights Part I**	**Bunsen-Hall**
13:00 - 13:20	Erik T. J. Nibbering (Max-Born-Institut, Berlin, Germany) From Local Covalent Bonding to Extended Electric Field Interactions in Proton Hydration	
13:20 - 13:40	Tabitha Amollo (Egerton University Nakuru, Kenya) Influence of materials characteristics on device performance: A case study of graphene-based nanomaterials in organic solar cells	
13:40 - 14:00	Qingsong Wang (University of Bayreuth/Bavarian Center for Battery Technology (BayBatt), Germany) High-entropy disordered rock-salt cathode for lithium-ion battery	
14:00 - 14:20	Tali Mass (University of Haifa, Israel) Primary coral polyps responses to decreasing seawater pH: observations from cell to the complete Organism	
14:20 - 14:40	Max Birch (RIKEN Center for Emergent Matter Science, Wako, Japan) Imaging stripes, skyrmions and higher-order spin textures in 2D magnets	
14:40 - 14:50	Jan-Dierk Grunwaldt - Committee Research with Synchrotron Radiation (KFS)	
14:50 - 15:20	Coffee Break	WISTA Foyer
15:20 - 16:20	**Bestowal of Prizes (EEK Prize & Innovation Award)**	**Bunsen-Hall**
16:20 - 17:00	**Science Highlights Part II - Science@MX Beamlines**	**Bunsen-Hall**
16:20 - 16:40	Jon Hughes (Justus-Liebig-Universität Giessen, Germany) Structure/function in phytochrome photoreceptors	
16:40 - 17:00	Irena Senkovska (Technische Universität Dresden, Germany) Metal-organic frameworks: from structure to function and *vice versa*	
17:00 - 17:15	**Welcoming Address by Ina Czyborra Senator for Higher Education and Research, Health, and Long-Term Care**	**Bunsen-Hall**
17:15 - 18:30	**Public Panel Discussion: "Science Diplomacy, International Collaboration and the Contribution of Lights Sources to Cooperative Solutions"**	**Bunsen-Hall**
from 18:30	**CURRYWURST & BEER**	**WISTA Foyer**

Programme Day 2 / 23 June 2023 / Friday		
08:30 - 14:30	Vendor Exhibition (all-day alongside the meeting)	WISTA Center
08:30 - 09:00	Registration	WISTA Foyer
09:00 - 09:30	Tobias Sontheimer (Helmholtz-Zentrum Berlin, Germany) HZB Energy Projects - CatLab, Care-O-Sene, Green Quest	Bunsen-Hall
09:30 - 10:45	**Young Scientists Session**	**Bunsen-Hall**
09:30 - 09:45	Jinzhao Li (Helmholtz-Zentrum Berlin, Germany) Rational Ink Design and Combinatorial Slot-Die Coating of Metal Halide Perovskites for Solar Cells	
09:45 - 10:00	David Sanchez-Manzano (CNRS-Thales, Palaiseau, France) Extremely long range, high-temperature Josephson coupling across a half metallic ferromagnet	
10:00 - 10:15	Frank Förste (Technische Universität Berlin, Germany) Quantitative Analysis and 2D/3D Elemental Imaging of Intact Cocoa Beans	
10:15 - 10:30	Pamela Morales Fernandez (MPI for Chemical Physics of Solids, Dresden, Germany) Imaging magnetization dynamics in three-dimensional magnetic nano double helices	
10:30 - 10:45	Building Bridges - Global Networking	
10:45 - 11:10	Coffee Break	WISTA Foyer
11:10 - 12:30	**Science Highlights Part III**	**Bunsen-Hall**
11:10 - 11:30	Rémi Dupuy (Sorbonne Université, Paris, France) Core-level photoelectron angular distributions at the liquid-vapor interface	
11:30 - 11:50	Maram Naes (Technische Universität Berlin, Germany) Across borders and scales: investigating Nabataean painted heritage at SESAME and BESSY II	
11:50 - 12:10	George E. Cutsail (MPI for Chemical Energy Conversion, Mühlheim, Germany) Applying VtC-XES to Obtain Oxidation-States of Organocopper Complexes	
12:10 - 12:30	Philipp Adelhelm (Humboldt Universität zu Berlin, Germany) Co-Intercalation Batteries (CoIBs): Role of TiS_2 as Electrode for Storing Solvated Na Ions	
12:30 - 13:30	Lunch Break	Canteens on-site
13:30 - 14:30	**POSTER SLAM**	**Bunsen-Hall**
14:30 - 15:00	Technical Break - Change of Location to BESSY II	
15:00 - 17:00	**POSTER SESSION**	**BESSY Exp. Hall**
from 17:00	**CELEBRATION - 25th Anniversary of BESSY II**	**BESSY Front Yard**

Abstracts of the Session - Science Highlights Part I

Thursday, 22 June 2023 from 13:00 to 14:50

Bunsen-Hall at WISTA Conference Center

From Local Covalent Bonding to Extended Electric Field Interactions in Proton Hydration

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Seemingly simple yet surprisingly difficult to probe, excess protons in water constitute complex quantum objects with strong interactions in the extended and dynamically changing hydrogen-bonding network of the liquid. Further elucidation of how protons are hydrated is crucially needed because of their pivotal roles in the von Grotthuss mechanism of proton transport in bulk aqueous media, in the transport mechanisms in energy conversion and signal transduction ranging from hydrogen fuel cells to transmembrane proteins. While geometries and stoichiometry have been widely addressed in both experiment and theory, the electronic structure of these specific hydrated proton complexes, however, has remained elusive to date. Here we show, layer by layer, how by utilizing novel flatjet technology for accurate x-ray spectroscopic measurements and with a combination of infrared spectral analysis and calculations, we find orbital-specific markers that distinguish two main electronic-structure effects: Local orbital interactions determine covalent bonding between the proton and neigbouring water molecules, while orbital-energy shifts measure the strength of the extended electric field of the proton. A hierarchy in electronic structure changes of water molecules involved in proton hydration, as evidenced by the local oxygen K-edge XAS contributions, is directly correlated with the strength of nearest neighbour hydrogen bond interactions and associated O···O distances.

References:

[1] Angew. Chem. Int. Ed. 61, e202211066 (2022)
[2] Angew. Chem. 134, e202211066 (2022)

Influence of materials characteristics on device performance: A case study of graphene-based nanomaterials in organic solar cells

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Solar energy is portentous in dealing with the ever-rising global demand for renewable, sustainable, and environmentally friendly energy resource. Emerging solar energy technologies such as organic solar cells (OSCs) and perovskite solar cells (PVSCs) are a cost-effective means of conversion of solar energy to electricity. Materials development and device engineering are requisite to effective solar energy conversion in these devices. This study reports the influence of materials characteristics on the prototype P3HT:PCBM solar cells. Graphene-based nanomaterials *viz*. graphene oxide (GO), reduced graphene oxide-germanium dioxide nanocomposite (rGO-GeO_2) and N-doped graphene-germanium quantum dots nanocomposite (GeQD/NGr) were employed in the photoactive medium of P3HT:PCBM solar cells. The inclusion of the nanomaterials in the photoactive layer yielded high short-circuit current densities (J_{sc}), which translated to improved power conversion efficiencies (PCEs) by up to 183%. The use of GO in the active layer remarkably improved the optical absorption leading to high charge carriers photogeneration requisite to high J_{sc}. GeQD/NGr in the active layer resulted in enhanced fill factor (FF). On the other hand, the devices with rGO-GeO_2 in the active layer exhibited decreased open-circuit voltage, V_{oc} and FF. rGO-GeO_2 and GeQD/NGr in the active layer blend served to ensure effective charge separation and transportation to the respective electrodes. Improved charge carrier mobilities were realized in all the devices with the nanomaterials in the active layers. Consequently, the study is a milestone in the quest for improved optical absorption and carrier mobilities in the photo active layer of OSCs.

References:

[1] Amollo T.A, Mola G.T and Nyamori V.O, Materials Chemistry and Physics, 254, 123448 (2020). doi:10.1016/j.matchemphys.2020.123448
[2] Amollo T.A, Mola G.T and Nyamori V.O, Solar Energy 171 83-91 (2018). doi:10.1016/j.solener.2018.06.068
[3] Amollo T.A, Mola G.T and Nyamori V.O, RSC Advances, 8, 21841-21849 (2018). doi:10.1039/C8RA04223C

High-entropy disordered rock-salt cathode for lithium-ion battery

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Traditional layered oxides consist of well-ordered alternating Li and transition metal (TM) with Li transport in two-dimensional (2D). In the disordered rock-salt (DRX) structure, Li and TM cations are randomly distributed at the 4a sites in the cationic sublattice [1]. The three-dimensional (3D) DRX cathodes are considerably more stable than the conventional layered oxides which often suffer from collapse of the interlayer spacing upon Li extraction at high voltages. The disordered arrangement of Li and TM opens the possibility of using a variety of TMs. The high-entropy DRX oxyfluorides, firstly reported by our group [2,3], of which the underlaying reaction mechanism has been intensively investigated recently especially by synchrotron-based techniques, including *operando* soft/hard X-ray absorption spectroscopy (XAS) and *ex situ* resonant inelastic X-ray scattering (RIXS).

References:

[1] Energy Environ. Sci. 13, 345–373 (2020)
[2] Energy Environ. Sci. 12, 2433–2442 (2019)
[3] Batter. Supercaps 3, 361–369 (2020)

Primary coral polyps responses to decreasing seawater pH: observations from cell to the complete organism

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In light of increasing stress and mass mortality of reef-building corals due to climate change, the resilience of some marine ecosystems relies on successful coral larva recruitment. Knowledge of the acclimatory and/or adaptive potential as a response to environmental challenges such as ocean acidification (OA) in the earliest life stages is limited. In this study, we report on *Stylophora pistillata* larvae and primary polyps cultured under acidic pH conditions. We investigated the response of the endosymbiotic algae and the coral host across biological levels, from cellular to organismal. By combining transcriptomic analysis with physiological and morphological measurements, we identified that while the number of survival and settlement of coral larvae were reduced under OA conditions, the surviving recruits adjusted well to the challenging conditions. Coupling synchrotron X-ray µCT with artificial intelligence, we found that OA has a morphologically-altering effect on coral skeletal features. Although skeleton growth is reduced, coral recruits possess acclimatory mechanisms allowing them to survive under OA conditions. These include the transition to a less-mineralized/increased-tissue phenotype exhibiting greater incorporation of organic matrix proteins within the skeletal fibers. Moreover, we found that the algal photosynthetic activity is stimulated under OA, as well as the transfer of photosynthates to the coral host, potentially sustaining the host energetic expenses.

Imaging stripes, skyrmions and higher-order spin textures in 2D magnets

Max T. Birch[1,2], Lukas Powalla[3], Kai Litzius[1,4], Sebastian Wintz[1,5], Frank Schulz[1], Fehmi Yasin[2], Luke A. Turnbull[6], Vanessa Nehruji[7], Ondrej Hovorka[7], Daniel Mayoh[8], Geetha Balakrishnan[8], Tanya Scholz[3], Bettina V. Lotsch[3], Markus Weigand[5], Xiuzhen Yu[2], Eberhard Goering[1], Klaus Kern[3], Marko Burghard[3], Gisela Schütz[1]

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The recently discovered two-dimensional (2D) magnets have become the focus of intense research [1,2]. Due to their atomically well-defined van der Waals interfaces, which lack dangling bonds, 2D magnets can be readily stacked with other 2D materials into heterostructures, allowing the exploitation of interlayer proximity effects [3]. These features confer 2D magnet-based devices with advantages over sputtered multilayers, which have already found widespread practical applications. Thus far, the magnetic structures hosted by 2D magnets have primarily been evaluated by electronic transport measurements, which, however, are often difficult to interpret. Therefore, we have utilized real-space imaging by scanning transmission x-ray microscopy performed at the MAXYMUS endstation at BESSY to investigate the spin textures found in a range of 2D magnets. In this talk, I will provide an overview of our observations of magnetic stripes, skyrmions and higher-order topological states [4-6]. We primarily studied exfoliated flakes of Fe_xGeTe_2, a family of 2D magnets with high Curie temperatures of up to 330 K. The results reveal valuable details of the magnetic interactions governing the magnetic structures in 2D magnets, and highlight the possibility of achieving and manipulating higher order topological textures in a wide range of magnetic systems.

References:

[1] K. S. Burch, et al. Nature 563, 47-52 (2018).
[2] C. Gong & X. Zhang. Science 363, eavv4450 (2019).
[3] M. Bora & P. Deb. J. Phys.: Mater. 4, 034014 (2021).
[4] M. T. Birch & L. Powalla, et al. Nat. Commun. 13, 3035 (2022).
[5] L. Powalla & M. T. Birch, et al. Nano Lett. 22, 9236-9243 (2022).
[6] L. Powalla & M. T. Birch, et al. Adv. Mater. 35, 2208930 (2023).

Abstracts of the Session - Science Highlights Part II / Science@MX Beamlines

Thursday, 22 June 2023 from 16:20 to 17:00

Bunsen-Hall at WISTA Conference Center

Structure/function in phytochrome photoreceptors

Jon Hughes, Soshi Nagano

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Phytochromes are photochromic biliprotein photoreceptors reversibly de/activated by red/far-red (R/FR) light. They are widely represented in micro-organisms including cyanobacteria, non-photosynthetic bacteria and certain fungi. In plants, however, they are ubiquitous, regulating thousands of genes through interactions with master transcription factors and thereby controlling such fundamental developmental processes such as seed germination, stem extension and day-length dependent flowering. Given the obvious ecological and agricultural importance of plant phytochromes, we and others strive to elucidate their action mechanism.

As the N-terminal photosensory module (comprising NTE, PAS, GAF and PHY domains) itself in plant phytochromes can signal autonomously, our work focuses on that *ca*. 60 kDa region of the molecule. The homologous region of cyanobacterial phytochrome Cph1 is particularly similar to that in plants, thereby providing a particularly tractable model for biophysical studies. Indeed, 2VEA, the 2.2 Å crystal structure of the wild-type Cph1 sensory module, was the first for a photoactive canonical phytochrome [1]. In the meantime, however, we have succeeded in solving the crystal structures of several phyB (6TC5, 6TL4, 6TBY) and phyA (6TC7) plant phytochrome constructs [2]. We now have an optimised 1.6 Å structure of the latter and moreover found that crystals of this construct are photochromic at room temperature. We have thus initiated serial X-ray crystallography experiments at European XFEL and T-REXX in Hamburg in collaboration with Manfred Weiss, Karsten Heyne and David von Stetten. Cph1 remains a valuable research object, however, not least for *in vivo* labelling, the Y176H [3] and Y263F [4] mutants showing fluorescence quantum efficiencies of *ca*. 14% and 8%, respectively [5]. We have now solved the crystal structure of Y176H to 3.7 Å and with the help of MAS NMR (Song; Uni Leipzig) and QM/MM calculations in both S0 and the S1 electronic excited state (Mackintosh & Schapiro; Jerusalem) revealed the origin of the enhanced fluorescence.

We gratefully acknowledge the assistance of Christian Feiler, Thomas Hauß, Frank Lennartz, Gert Weber and Manfred Weiss in our work at the BESSY II MX beamlines operated by the *Helmholtz-Zentrum Berlin für Materialien und Energie*.

References:

[1] Essen, Mailliet & Hughes (2008) PNAS.
[2] Nagano, Guan, Shenkutie, Feiler, Weiss, Kraskov, Buhrke, Hildebrandt & Hughes (2020) Nature Plants.
[3] Fischer & Lagarias (2004) PNAS.
[4] Mailliet, Psakis, Feilke, Sineshchekov, Essen & Hughes (2011) JMB.
[5] Nagano, Sadeghi, Balke, Fleck, Heckmann, Psakis & Alexiev (2022) Sci. Reports.

Metal-organic frameworks: from structure to function and *vice versa*

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An essential requirement to develop new functional materials for chemical conversion and separation is the design of materials with a high degree of crystallinity, providing uniform porosity and atomically precise positioning of active sites in the pore interior. Metal-Organic Frameworks (MOFs), or porous coordination polymers (PCPs), are crystalline materials in which the pore size and functionality can be tailored by choice of the building blocks and their connectivity. Based on these rational design principles, MOFs have rapidly evolved as novel platform for diverse applications.

The materials rationally designed and developed at Dresden University of Technology (DUT) show superior properties in terms of porosity and function [1-4].

High specific surface area and pore volume are needed for effective high-pressure gas storage. The strategy, which enabled the remarkable increase of the specific surface area and pore volume from 2.02 cm^3/g in DUT-6 [1] to 5.05 cm^3/g in DUT-60 [2], will be presented. DUT-60 is the MOF with the worldwide highest specific surface area, pore volume, and hydrogen storage capacity.

The second part of the presentation will highlight the guest-induced structural flexibility in MOFs and its advantages over rigid adsorbents, such as the improved gas separation performance of DUT-8(Ni) [3]. The novel, counterintuitive negative gas adsorption (NGA) phenomenon discovered in mesoporous DUT-49 MOF and based on single-crystal to single-crystal structural transition will be discussed [5].

References:

[1] N. Klein, I. Senkovska, K. Gedrich, U. Stoeck, A. Henschel, U. Mueller, S. Kaskel, Angew. Chem. Int. Ed., 48, 9954 (2009).
[2] I. M. Hönicke, I. Senkovska, V. Bon, I. A. Baburin, N. Bönisch, S. Raschke, J. D. Evans, S. Kaskel, Angew. Chem. Int. Ed., 57, 13780 (2018).
[3] I. Senkovska et al., Angew. Chem. Int. Ed., DOI 10.1002/anie.202218076 (2023).
[4] V. Bon, S. Krause, I. Senkovska, N. Grimm, D. Wallacher, D. M. Többens, S. Kaskel, Angew. Chem. Int. Ed., 60, 11735 (2021).

Abstracts of the Young Scientists Session

Friday, 23 June 2023 from 09:30 to 10:45

Bunsen-Hall at WISTA Conference Center

Rational Ink Design and Combinatorial Slot-Die Coating of Metal Halide Perovskites for Solar Cells

Jinzhao Li[1,2], Oleksandra Shargaieva [1], Natalia Maticiuc [1], Janardan Dagar[1], Marco Remec,[1] Quiterie Emery,[1] Mark Khenkin,[1] Hans Köbler,[1] Daniel M. Többens,[1] Ivo Zizak,[1] Emil J. W. List-Kratochvil,[1,2] and Eva Unger[1,2]

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Metal-halide perovskite semiconductors are of interest for various optoelectronic devices: photovoltaics, light-emitting diodes, lasers, and photodetectors [1]. These materials can be processed from solutions on large areas using slot-die coating method. First, a methylammonium lead iodide ($MAPbI_3$) based perovskite precursor ink based on 2-methoxyethanol (2-ME) was optimized with respect to the appropriate amounts of dimethylsulfoxide (DMSO) used as a solvent additive. The origin of performance differences was rationalized by performing in-situ Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) and Small Angle X-ray Scattering (SAXS) measurements during film formation [2]. Second, we investigated the effect of acetonitrile (ACN) in a 2-ME solvent based on formamidinium lead triiodide ($FAPbI_3$) perovskite. The ink viscosity was adjusted by using ACN as a co-solvent leading to high quality $FAPbI_3$ thin-films. For an optimized content of 46 vol% of the ACN co-solvent, a certified steady-state performance of 22.3% was achieved [3]. In addition, we employed a combinatorial slot-die coating method to fabricate perovskite of compositions from $FAPbI_3$ to $MAPbBr_3$. To characterize the homogeneity and quality of samples, we carried out ex situ-GIWAXS mapping of films. It highlights a high-throughput strategy for screening and exploring the compositional and structural properties of metal halide perovskite semiconductors [4].

This work will present results spanning from fundamental in-situ XRD studies during halide perovskite growth carried out at the BESSY II synchrotron light source, to controlling the thin-film layer homogeneity by rational ink design, to making high-performance small and larger area solar cell prototypes.

References:

[1] ACS Energy Lett., 7, 2084–2091(2022)
[2] Adv. Energy Mater. 11, 2003460 (2021)
[3] Adv. Energy Mater. 16146840 (2023)
[4] Res. Sq., https://doi.org/10.21203/rs.3.rs-2800085/v1, (2023)

Extremely long range, high-temperature Josephson coupling across a half metallic ferromagnet

D. Sanchez-Manzano[1,2], S. Mesoraca[2], F. Cuellar[1], M. Cabero[3,4], V. Rouco[1], G. Orfila[1], X. Palermo[2], A. Balan[2], L. Marcano[5], A. Sander[2], M. Rocci[1,†], J. Garcia-Barriocanal [6], F. Gallego[1], J. Tornos[1], A. Rivera[1], F. Mompean[7,8], M. Garcia-Hernandez [7,8], J. M. Gonzalez-Calbet[4,9], C. Leon[1], S. Valencia[5], C. Feuillet-Palma[10], N. Bergeal[10], A. Buzdin[11], J. Lesueur[10], Javier E. Villegas[2,*], J. Santamaria[1,8]

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The Josephson effect results from the coupling of two superconductors across a non-superconducting spacer to yield a quantum coherent state. In ferromagnets, singlet (opposite-spin) Cooper pairs decay over very short distances, and thus Josephson coupling requires a nanometric spacer. In specific systems, however, equal spin triplet Cooper pairs can be generated, allowing the coupling of superconductors across magnetic barriers over much longer distances. Despite many experimental hints of triplet superconductivity at ferromagnet/superconductor interfaces, long range triplet Josephson effects across ferromagnetic barriers have remained elusive. We demonstrate extremely long-range high-temperature Josephson coupling across the half-metallic manganite $La_{0.7}Sr_{0.3}MnO_3$ combined with the superconducting cuprate $YBa_2Cu_3O_7$ [1,2]. We study the origin of this proximity effect by observing the magnetic behavior of LSMO both by transport and XMCD measurements. YBCO/LSMO planar junctions display the hallmarks of Josephson physics: critical current oscillations (Fraunhofer pattern) and quantum phase locking under microwave excitation (Shapiro steps). The marriage of high-temperature quantum coherent transport and full spin polarization brings unique opportunities for the practical realization of superconducting spintronics, and enables novel strategies for devices in quantum technologies.

References:

[1] D. Sanchez-Manzano, et al. Nat. Mater. 21, 188–194 (2022).
[2] D. Sanchez-Manzano et al. Supercond. Sci. Technol. (2023) (accepted)

Quantitative Analysis and 2D/3D Elemental Imaging of Intact Cocoa Beans

Frank Förste[1], Leona Bauer[1], Cornelia Streeck[2], Martin Radtke[3], Uwe Reinholz[3], Daniel Kadow[4], Claudia Keil[5], Ioanna Mantouvalou[6]

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As an important raw material for the confectionery industry, the cocoa bean (Theobroma cacao L.) must meet certain legal requirements in terms of food safety and maximum contaminant levels in order to enter the cocoa market. Understanding the enrichment and distribution of essential minerals but also toxic metals is of utmost importance for improving the nutritional quality of this economically important raw food material.

To analyze the elemental composition and distribution of cocoa beans X-ray fluorescence (XRF) techniques are predestined. We present XRF techniques for elemental bio-imaging of intact cocoa beans to localize minerals and minor constituents and an additional XRF technique for quantitative analysis of cocoa pellets. The interrelation of all the methods presented gives a detailed picture of the content and 3D-resolved distribution of elements in complete cocoa beans for the first time [1].

Reference:

[1] Anal. Chem. 95, 13, 5627-5634 (2023)

Imaging magnetization dynamics in three-dimensional magnetic nano double helices

I. Pamela Morales Fernández[1], Sandra Ruiz Gómez[1], Claudia Fernández González[1], Elina Zhakina[1], Markus König[1], Aurelio Hierro Rodríguez[2,3], Simone Finizio[4], Sebastian Wintz[5], Claas Abert[6], Dieter Suess[6], Amalio Fernández Pacheco[7,8], Claire Donnelly[1]

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The extension of nanomagnetism from two dimensions provides exciting opportunities to go beyond the physics of planar systems, with prospects for new topological textures, curvilinear effects, and complex magnetization dynamics [1],[2]. Here, we experimentally explore the physics of magnetic double helix nanostructures, three-dimensional systems that host an exotic magnetic configuration composed by pairs of highly coupled domain walls. These bound domain wall pairs arise from the natural competition between intrastructural properties (e.g., shape anisotropy and chirality) and magnetostatic inter-helix interactions, resulting in the formation of topological textures in the magnetic induction [3]. Beyond the static configuration, three dimensional chiral systems are predicted to exhibit rich dynamical processes [4],[5]. In this talk I will present the direct mapping of magnetization dynamics within the double helix nanostructure [6]. Specifically, we harness three-dimensional nanofabrication techniques [7] to fabricate cobalt nano double helices onto striplines, to apply high frequency field excitations. By preforming time-resolved scanning transmission X-ray microscopy [8] at the MAXYMUS beamline, we map the dynamics response of the coupled domain walls, revealing localized dynamics in the double helix conduit. These first results establish the study of the dynamics of three-dimensional magnetic nanostructures, opening the door to complex dynamics in three dimensional geometries.

References:

[1] Fernández Pacheco, et al. Nat. Commun., 8:15756 (2017).
[2] S. Da Col, et al. PRB. 89, 180405 (2014).
[3] Donnelly, et al. Nat. Nanotechnol. 17, 136–142 (2022).
[4] M. Yan, et al. APL 100, 252401 (2012).
[5] Sánz-Hernández, et al. ACS Nano 2020, 14, 8084-8092 (2020).
[6] Donnelly, et al. J. Phys.: Condens. Matter, 32 213001 (2020).
[7] L. Skoric, et al. Nano Lett. 20, 1, 184–191 (2020).
[8] C. Donnelly, Nat Nanotechnol. 15(5):356-360 (2020).

Abstracts of the Session - Science Highlights Part III

Friday, 23 June 2023 from 11:10 to 12:30

Bunsen-Hall at WISTA Conference Center

Core-level photoelectron angular distributions at the liquid-vapor interface

Rémi Dupuy[1,2], J. Filser[1], C. Richter[1], T. Buttersack[1], F. Trinter[1,3], S. Gholami[1], R. Seidel[4], C. Nicolas[5], J. Bozek[5], H. Oberhofer[6], S. Thürmer[7], U. Hergenhahn[1], K. Reuter[1], B. Winter[1] and Hendrik Bluhm[1]

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3 Institut für Kernphysik, Goethe-Universität, Frankfurt am Main, Germany
4 Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany
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6 Department of Physics, University of Bayreuth, Bayreuth, Germany
7 Department of Chemistry, Kyoto University, Kyoto, Japan

Photoelectron spectroscopy (PES) has turned into a powerful tool for the investigation of liquid−vapor interfaces. Liquid-vapor (especially aqueous-vapor) interfaces play a major role in atmospheric science, for example in the interaction of oceans with the atmosphere, in aqueous aerosols where they govern important chemical reactions, or in the evaporation of lakes and reservoirs. PES offers a surface-sensitive and chemically sensitive probe at the molecular scale, allowing to investigate the specific composition and structure of the first few nanometers into the liquid. Quantitative analysis of the signals to retrieve the depth structure of these first nanometers is however difficult.

Through some recent experiments [1-4], we will show here how the measurement of the angular distribution of the photoelectrons provides precious additional information that helps disentangle this problem. Angular distributions are modified by elastic scattering of the photoelectrons during their transport to the surface. This modification is depth-dependent and thus can be used to retrieve depth information, with a remarkable resolution down to 1 Å.

References:

[1] Dupuy, R.; Thürmer, S.; Richter, C.; Buttersack, T.; Trinter, F.; Winter, B.; Bluhm, H. Acc. Chem. Res. 2023, acs.accounts.2c00678.
[2] Dupuy, R.; Filser, J.; Richter, C.; Buttersack, T.; Trinter, F.; Gholami, S.; Seidel, R.; Nicolas, C.; Bozek, J.; Egger, D.; Oberhofer, H.; Thürmer, S.; Hergenhahn, U.; Reuter, K.; Winter, B.; Bluhm, H. Phys. Rev. Lett. 2023, 130 (15), 156901.
[3] Dupuy, R.; Filser, J.; Richter, C.; Seidel, R.; Trinter, F.; Buttersack, T.; Nicolas, C.; Bozek, J.; Hergenhahn, U.; Oberhofer, H.; Winter, B.; Reuter, K.; Bluhm, H. Phys. Chem. Chem. Phys. 2022, 24 (8), 4796–4808.
[4] Lewis, T.; Winter, B.; Thürmer, S.; Seidel, R.; Stephansen, A. B.; Freites, J. A.; Tobias, D. J.; Hemminger, J. C. J. Phys. Chem. C 2019, 123 (13), 8160–8170.

Across borders and scales: investigating Nabataean painted heritage at SESAME and Bessy II

Maram Naes

Institute for Optics and Atomic Physics, Technical University Berlin, Germany

Nabataean wall paintings from the UNESCO World Heritage Site of Petra in Jordan are unique surviving evidence for Nabataean painted materials and technology. We aim at understanding these paintings by investigating their composition and painting technology using non-invasive and non-destructive lab and synchrotron microscopic and spectroscopic methods. A first journey from Petra (Jordan) to Berlin (Germany) took place over a decade ago to investigate the paintings at TUB and Bessy II. Results allowed successful identification of elemental and chemical composition of the various paint layers. However, molecular investigations led us to another journey from Berlin (Germany) to Allan (Jordan) where EMIRA beamline at SESAME synchrotron opened its doors for studying the Nabataean painted heritage. We present a selection of the results from our experiments at the lab and synchrotron facilities.

References:

[1] Naes, M., *et al.* (2012). 8th SESAME Users Meeting
[2] Naes, M., *et al.* (2019). 17th SESAME User Meeting

Applying VtC-XES to Obtain Oxidation-States of Organocopper Complexes

George E. Cutsail III[1,2], Blaise L. Geoghegan[1,2], Yang Liu[3], Sergey Peredkov[1], Sebastian Dechart[3], Franc Meyer[3], Serena DeBeer[1]

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3 Institute of Inorganic Chemistry, University of Göttingen, Germany

Valence-to-Core (VtC) X-ray Emission Spectroscopy (XES) is a rapidly developing tool with numerous applications in various molecular chemistry, biological, and catalytic systems. This core spectroscopy is particularly sensitive to ligand identity, bond length, molecular orbital structure and geometry. Complementing the core excitations to unoccupied orbitals in X-ray absorption spectroscopy (XAS), VtC XES directly probes the filled valence shell through the emission transitions. While XAS is generally accepted as sensitive probe of oxidation-state, VtC XES's sensitivity to oxidation-state is less described.

During this talk, I will discuss our recent work to characterize a series of macrocyclic organometallic copper complexes in formal oxidation states ranging from +1 to +3 by a combination of Cu K-edge XAS and VtC XES. The observed transitions will be placed in context of their electronic structure and supported by DFT calculations. We have extended these methods to the study of the $[Cu(CF_3)_4]^-$ ion and its hotly debated oxidation-state. Combining XAS and VtC XES further demonstrates the necessity of combining multiple spectroscopies when investigating the electronic structures of highly covalent copper complexes, providing a template for future investigations into both synthetic and biological metal centers.

Both the current research of the PINK X-ray emission beam line and other joint instrument development plans in the field of XES by the Max Planck Institute for Chemical Energy Conversion and HZB will also be highlighted.

Reference:

[1] J Am Chem Soc 144, 2520–2534 (2022)

Abstracts of the Poster Slam

Friday, 23 June from 13:30 to 14:30

Bunsen-Hall at WISTA Conference Center

In the order of appearance:

Time-resolved X-ray diffraction (TR-XRD) studies on ferroelectric thin film

Rekikua Alemayehu (Universität Potsdam)

Polarization switching in ferroelectrics involves the motion of atoms in the crystal structure. TR-XRD is a powerful technique to study the structural changes during this process. Here, we show simultaneous structural and electrical responses during and after the application of periodic pulses and discuss how the transient strain encodes the influence of imprint phenomena on the switching dynamics.

Molecular Pathomechanisms in Lipoamide Dehydrogenase Deficiency

Attila Ambrus (Semmelweis University)

Crystal structures of the human lipoamide dehydrogenase, the common third component (E3) to the mitochondrial alpha-keto acid dehydrogenases, and nine of its pathogenic variants were determined at 1.44 - 2.89 Å resolutions to analyze the structural bases of the often prematurely lethal E3 deficiency. Perturbations were found in the active site, the cofactor binding sites, and/or the H^+/H_2O channel.

Going operando: Testing Solid-State Anode-free Lithium-Metal Batteries

Zora Chalkley (Helmholtz-Zentrum Berlin)

In anode-free lithium (Li) metal batteries (AFLMBs), Li metal is plated on a current collector degrading the electrode/electrolyte interface forming intermediates that we propose to probe with operando hard x-ray photoelectron spectroscopy (HAXPES). The range of information obtainable is presented herein. The impact of this data analysis is demonstrated by comparison of solid polymer electrolytes.

Structural properties of silver sulfide-reduced graphene oxide nanocomposite

Robert Ngure (Egerton University)

This paper reports the structural analysis of silver sulfide-reduced graphene oxide (Ag_2S-rGO) nanocomposite synthesized by chemical reduction method. SEM confirmed the formation of the nanocomposite by showing that rGO sheets were intercalated in Ag_2S nanoparticles and that Ag_2S had the shape of nanowires. X-ray diffraction revealed a d spacing ranging between 1.0 Å and 5.2 Å.

Monitoring the Formation of Nickel-Poor and Nickel-Rich Oxide Cathode Materials for Lithium-Ion Batteries with Synchrotron Radiation

Ying Bixian (Universität Münster)

The syntheses of Ni-poor (NCM111) and Ni-rich (NCM811) lithium transition-metal oxides are investigated using in situ synchrotron powder diffraction and near-edge X-ray absorption fine structure spectroscopy. he synthesis of NCM811 incorporates an intermediate phase with a rock salt-type structure, whereas NCM111 maintains a layered structure throughout the entire synthesis process.

Hydroxide based High Entropy Metal Organic Framework for Oxygen Evolution Reaction

Arkendu Roy (Bundesanstalt für Materialforschung und -prüfung)

High entropy metal hydroxide organic frameworks (HE-MHOFs) are composed of high entropy hydroxide layer inside MOFs, resulting in a high degree of structural complexity and diversity than conventional MOFs. It exhibits outstanding performance towards oxygen evolution reaction (OER) comparable to benchmark catalysts like IrO_2 and platinum carbon.

Development of tender X-ray multilayer coated gratings operating at high diffraction order

Yeqi Zhuang (Tongji University)

In the tender x-ray range, operating multilayer coated grating at high diffraction order is highlighted to improve transmission and energy resolution of grating-based beamline/spectrometer. Two samples have an experimental efficiency of 12% - 34% at 2.5 keV at the 2^{nd} - 4^{th} order what is above 10~30 times higher than Au coated grating. The experimental angular dispersion shows a good agreement with the theory.

ReMade@ARI - a hub for materials research for the circular economy

Lakshmi Bhaskaran (Helmholtz-Zentrum Dresden-Rossendorf)

ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Research Infrastructures) is committed to the development of innovative and sustainable materials for the circular economy. The project provides scientists from academia and industry exploring the properties and structures of recyclable materials with coordinated access to more than 50 analytical research infrastructures across Europe.

Surface and bulk chemical imaging of $Ti_3C_2T_x$ MXenes by scanning X-ray microscopy

Faidra Amargianou (Helmholtz-Zentrum Berlin)

MXenes are layered two-dimensional materials with outstanding properties for electrochemical energy storage. Their surface chemistry can be tuned during synthesis. We introduce scanning X-ray microscopy with simultaneous transmission and electron yield detection, enabling chemical imaging with bulk and surface sensitivity, respectively, of individual MXene flakes.

Visualization of Deep discharge mechanism using operando XCT

Shahabeddin Dayani (Bundesanstalt für Materialforschung und -prüfung)

Thanks to their high brilliance, synchrotron beam facilitates us to do a full Computed Tomography in a short time. This enables us to measure batteries while being cycled with a reasonable time resolution to record morphological changes. In this presentation we illustrate how one can utilize this ability to investigate abuse mechanisms on an actual commercially available lithium-ion battery from cell level.

The Role of PEIE as a Functionalizing Layer for Hybrid Perovskite/Si Tandem Devices

Elif Hüsam (Helmholtz-Zentrum Berlin)

We studied metal halide perovskites (HaPs) used as photoactive absorber layers in tandem solar cells and their buried interface with an evaporated C_{60} electron transport layer (ETL). The effect of interface engineering via the inclusion of a PEIE interlayer was probed by HAXPES. We present the chemical and electronic properties of the C_{60} /HaP interface as a function of a PEIE interlayer.

Morphological features and electrical properties of hollow SnO_2 for room temperature CO sensing

Bridget Mutuma (University of Nairobi)

This study highlights the synthesis of hollow SnO_2 nanostructures and their physicochemical properties. Hollow SnO_2 structures were utilized in the sensing of CO at room temperature and the sensor response was found to be six times higher than that of the solid SnO_2. This study indicated that the hollow SnO_2 obtained from a SiO_2 core-shell template has the potential to become a viable sensor material for CO.

Surface-mediated Charge Transfer of Photogenerated Carriers in Diamond

Arsène Chemin (Helmholtz-Zentrum Berlin)

Despite a large bandgap of 5.5 eV, charge carriers in diamond can be excited by visible light due to the presence of surface states. These transitions are identified using a combination of X-ray and UV/Vis spectroscopic techniques, providing a new understanding of the sub-bandgap photocurrent observed with diamond electrodes, which could enable visible light-driven photoelectrochemical CO_2 and N_2 reduction.

Unravelling the Effect of Pt isolation on shallow d-states of Gallium-Platinum Alloys

Tzung-En Hsieh (Helmholtz-Zentrum Berlin)

The properties of in-system prepared SiOx-supported GaPt alloys is examined by energy-dependent PES exploiting EMIL's two-color beamline. Pt isolation results in a narrowing and shift of the Pt 5d-derived band. Liquefaction, oxidation, and reduction of GaPt alloys with 1 at % Pt induces a surface enrichment of Pt and the formation of new phases, presumably representing the active catalyst surface.

Electronic Structure of the Complete Series of Gas Phase Manganese Acetylacetonates by X-ray Absorption Spectroscopy

Olesya Ablyasova (Helmholtz-Zentrum Berlin)

We have performed X-ray absorption spectroscopy (XAS) in ion yield mode at the manganese L-edge and oxygen and carbon K-edge on a series of gas-phase mass-selected $Mn(acac)^+_n$ (n=1-3). Accompanied by RAS/DFT calculation and CF/CT modeling, we are able to extract information about the geometry, electronic structure, spin and oxidation state of the $Mn(acac)^+_n$.

Long-periodic spin textures in vector magnetic fields as seen by resonant elastic x-ray scattering at VEKMAG

Victor Ukleev (Helmholtz-Zentrum Berlin)

Resonant elastic small-angle soft x-ray scattering (REXS) is the unique tool to study long-periodic spin textures in noncentrosymmetric magnets with unprecedented reciprocal-space resolution. The vector-field installation VEKMAG at PM-2 allows to probe such spin spirals at cryogenic temperatures and vector magnetic fields providing unique parameters of spin Hamiltonian hitherto unavailable by other probes.

Abstracts of the Poster Session

Friday, 23 June from 15:00 to 17:00

BESSY II Experimental Hall

0 f Long-term Degradation Mechanisms in Application-Implemented Radical Thin Films

Ewa Nowik-Boltyk (Universität Tübingen)

Blatter radical derivatives are very attractive due to their potential applications, ranging from batteries to quantum technologies. We focus on the latest insights regarding the fundamental mechanisms of radical thin film long-term degradation by comparing two Blatter radical derivatives.

0 g Magnetic nanodoping: Stern-Gerlach deflection and x-ray magnetic circular dichroism

Vicente Zamudio-Bayer (Helmholtz-Zentrum Berlin)

We have investigated the interaction between a magnetic impurity and a nanoscale non-magnetic host via molecular beam and ion trapping techniques on free, cobalt-doped silver clusters. Using both techniques allowed us to investigate both neutral and cationic clusters and also gave us access to two magnetic relaxation regimes: internal vibrational and buffer gas collision-assisted relaxation.

1 Electronic Structure of the Complete Series of Gas Phase Manganese Acetylacetonates by X-ray Absorption Spectroscopy

Olesya Ablyasova (Helmholtz-Zentrum Berlin)

We have performed X-ray absorption spectroscopy (XAS) in ion yield mode at the manganese L-edge and oxygen and carbon K-edge on a series of gas-phase mass-selected $Mn(acac)^{+}_{n}$ (n=1-3). Accompanied by RAS/DFT calculation and CF/CT modeling, we are able to extract information about the geometry, electronic structure, spin and oxidation state of the $Mn(acac)^{+}_{n}$.

2 Quantifying energy shifts in transition metal model systems with high resolution x-ray spectroscopy beyond the oxidation state

Max Flach (Helmholtz-Zentrum Berlin)

In this study we provide a systematic investigation of changes in the iron and nickel L-edge excitation energy depending on the charge distribution on the metal center of gas phase diatomic FeX^{+} and NiX^{+} (X = F, Cl, Br, I), as well as monoatomic cations in different electronic configurations using high resolution x-ray absorption spectroscopy.

4 Exploring electronic properties of Copper(Cu) via Auger Photoelectron Coincidence Spectroscopy

Swarnshikha Sinha (Helmholtz Zentrum Berlin)

Auger-Photoelectron-Coincidence Spectroscopy (APECS) provides unprecedented selectivity to determine in mixed valence materials the contributions of the underlying electronic configuration. We with APECS, studied three different Copper (Cu) surfaces at the CoESCA endstation, UE52-PGM beamline, BESSYII and could visualize substantial differences in the screening of the final states of the three Cu surfaces.

4 b 30 Tesla Pulsed Magnetic Field Station at UE46

Oleksandr Prokhnenko (Helmholtz-Zentrum Berlin)

A pulsed magnetic field station at UE46 is presented. It is dedicated to soft x-ray absorption measurements in fields up to 30 T. Central part of the station is a liquid-nitrogen cooled 30 T solenoid magnet driven by a capacitor bank of C = 6.4 mF. The magnet pulse length amounts to 4 ms and the repetition rate at 30(10) T to 5(1) min. We present technical characteristics of the station and selected results

7 Surface and bulk chemical imaging of $Ti_3C_2T_x$ MXenes by scanning X-ray microscopy

Faidra Amargianou (Helmholtz-Zentrum Berlin)

MXenes are layered two-dimensional materials with outstanding properties for electrochemical energy storage. Their surface chemistry can be tuned during synthesis. We introduce scanning X-ray microscopy with simultaneous transmission and electron yield detection, enabling chemical imaging with bulk and surface sensitivity, respectively, of individual MXene flakes.

8 The Maxymus STXM at BESSY II

Sebastian Wintz (Helmholtz-Zentrum Berlin)

We will provide an introduction to the Maxymus state-of-the-art Scanning Transmission X-ray Microscope (STXM) at BESSY II. We will focus on recent technical and scientific advances, such as magnetic imaging in 2D van-der-Waals materials, high-frequency time-resolved measurements up to 40 GHz, and an improved time-resolved data acquisition.

32 One-dimensional electronic structure of phosphorene chains

Maxim Krivenkov (Helmholtz-Zentrum Berlin)

Using angle-resolved photoemission we studied P atomic chains self-assembled on Ag(111). P electronic bands dispersionless perpendicular to the wire reveal a 1D confinement of electrons. Our density functional calculations, apart from precise reproduction of the 1D P band, predict a 1D to 2D metallic transition in the electronic structure upon increasing density of the atomic chains array.

34 EPIC Monday-Morning Integration

Florin Boariu (Helmholtz-Zentrum Berlin)

A most frustrating challenge while performing experimental measurements ("beamtime") as a synchrotron guest is integrating new gadgets into the local experiment orchestration system. We introduce EMMI, an emerging Python framework aimed at rapid device integration into EPICS-controlled environments. The driving idea is not to just do it "faster"; it's to do it on the first day before lunch.

35 Time-resolved wide-energy operando-XAS on catalysis at KMC-3

Michael Haumann (Freie Universität Berlin)

A versatile setup for X-ray absorption spectroscopy at KMC-3 provides rapid-scan (5 s), time-resolved (1 ms), energy-resolving (13-element SDD), operando (electrochemistry) and cryo (closed-cycle He cryostat), and light-excitation (OPO ns-laser) facilities for experiments in a wide energy range (2-15 keV and perhaps 21 keV soon) for investigations on bio/chemical catalysts, proteins, and battery materials.

38 A time-domain perspective on the structural and electronic response in epitaxial ferroelectric thin films

Matthias Rössle (Helmholtz-Zentrum Berlin)

Using synchrotron-based time-resolved X-ray diffraction, we investigate the frequency-dependent operando response of epitaxially grown $Pb(Zr_{0.48}Ti_{0.52})$ test capacitors integrated on Silicon substrates. We find that the electrical and structural hystersis loops deform at high frequencies leading to a lower polarization, which we explain in the time-domain using a simplified Duffing oscillator model.

39 Time-resolved X-ray diffraction (TR-XRD) studies on ferroelectric thin film

Rekikua Alemayehu (Universität Potsdam)

Polarization switching in ferroelectrics involves the motion of atoms in the crystal structure. TR-XRD is a powerful technique to study the structural changes during this process. Here, we show simultaneous structural and electrical responses during and after the application of periodic pulses and discuss how the transient strain encodes the influence of imprint phenomena on the switching dynamics.

40 Examination of charge carrier dynamics and their influence on mechanical curvature in a highly strained bent single $Al_xIn_{1-x}As$/GaAs core shell nanowires as function of diameter via optical excitation using laser pump and X-ray probe method

Taseer Anjum (Universität Siegen)

Presence of a gradient in bandgap in bent nanowires modifies the dynamics of excited charge carriers, resulting in significant changes in mechanical and thermal properties. Variation in the bending radius of bent nanowires is detectable via a shift of the diffraction peak in reciprocal space. The study will contribute to our understanding of the piezoelectric and flexoelectric responses at the nanoscale.

45 Oxadiazole-based inhibitors of histone deacetylase 6 are hydrolyzed upon enzyme engagement

Lucia Motlová (Czech Academy of Sciences)

Zinc-dependent histone deacetylases (HDACs) play critical roles in many pathophysiological processes and thus serve as targets of therapeutics in cancers and neurological diseases. HDAC inhibitors typically contain a hydroxamate zinc-binding group (ZBG). Alternative ZBGs can improve selectivity and ADMET profiles. We co-crystallized HDAC6 and an oxadiazole-based inhibitor to see their interaction.

46 Molecular Pathomechanisms in Lipoamide Dehydrogenase Deficiency

Attila Ambrus (Semmelweis University)

Crystal structures of the human lipoamide dehydrogenase, the common third component (E3) to the mitochondrial alpha-keto acid dehydrogenases, and nine of its pathogenic variants were determined at 1.44 - 2.89 Å resolutions to analyze the structural bases of the often prematurely lethal E3 deficiency. Perturbations were found in the active site, the cofactor binding sites, and/or the $H+/H_2O$ channel.

47 Investigation of the elemental distributions in honey bees and honey bee larvae by X-ray fluorescence spectroscopy

Yannick Wagener (Technische Universität Berlin)

Current research shows that the trace element zinc could have a positive effect on the immune system of honey bees and other insects. For a better understanding of the bio activity of zinc, honey bees with a zinc enriched diet were examined. With the help of micro X-ray fluorescence spectroscopy (µXRF), two- and three-dimensional images of the elemental distributions inside the honey bees could be obtained.

49 Alice II, a new instrument for resonant magnetic scattering, coherent magnetic imaging and magnetization dynamics with synchrotron radiation

Florin Radu (Helmholtz-Zentrum Berlin)

Alice II instrument has been developed, commissioned and made available for user experiments in the last 5 years, within the BMBF project No. 05K19WO6. It extends the experimental capabilities of the former Alice instrument, like soft x-ray reflectivity and spectroscopy, with new scattering capabilities at large incident angles and for large reciprocal spaces.

51 Helmholtz Digital Research Infrastructure: ROCK-IT

Britta Höpfner (Helmholtz-Zentrum Berlin)

Insights into "catalysts at work" are of high interest, prompting the ROCK-IT project partners DESY, HZB, HZDR and KIT to enhance capabilities for in situ and operando experiments by optimizing development workflows through common protocols, standards, automation, robotics, and AI usage thereby lowering access barriers for non-expert users and industry and accelerating innovation cycles.

52 SECoP and SECoP@HMC - Metadata in the Sample Environment Communication Protocol

Klaus Kiefer (Helmholtz-Zentrum Berlin)

The Sample Environment Communication Protocol (SECoP) was developed to standardize the communication between instrument control software and sample environment (SE) equipment. SECoP offers a generalized way to control SE equipment and transports SE metadata in a well-defined way. Here we present SECoP and the SECoP@HMC project supported by the Helmholtz Metadata Collaboration (HMC).

53 Helium Management at HZB

Bastian Klemke (Helmholtz-Zentrum Berlin)

HZB is developing solutions for Helium Management, which enable us to monitor and control the liquid and gaseous Helium on both campuses. Helium is a limited resource, which has seen an incredible increase in price. The current shortage of Helium on the global market led to significant problems for the realization of planned experiments. Therefore, we have to control and reduce the losses of Helium.

61 Blazed Soft X-Ray Gratings Fabricated by Grey-Tone Electron-Beam Lithography and Thermal Oxidation of Silicon

Nazanin Samadi (Paul Scherrer Institute)

We report on a novel method for the production of next-generation blazed soft X-ray gratings based on grey-tone electron-beam lithography and thermal oxidation of silicon. The fabrication process along with the at-wavelength characterization of manufactured blazed gratings will be presented. The initial gratings show high efficiency and very low diffuse scattering noise.

62 Highly efficient multilayer-coated gratings for tender X-ray energy range

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.

63 Next generation blazed grating by grey-tone e-beam lithography

Analía Fernández Herrero (Helmholtz-Zentrum Berlin)

E-beam lithography is being explored as an alternative to ruling for the production of blazed profile gratings. It is a versatile tool that allows patterning of large areas in a relatively short time. To ultimately establish a reliable method for the fabrication of future smart gratings, a systematic analysis is needed. Here, we report on the on-going investigations and production of such gratings.

64 Development of tender X-ray multilayer coated gratings operating at high diffraction order

Yeqi Zhuang (Tongji University)

In the tender x-ray range, operating multilayer coated grating at high diffraction order is highlighted to improve transmission and energy resolution of grating-based beamline/spectrometer. Two samples have an experimental efficiency of 12% - 34% at 2.5 keV at the 2^{nd} - 4^{th} order what is above 10~30 times higher than Au coated grating. The experimental angular dispersion shows a good agreement with the theory.

65 The Role of PEIE as a Functionalizing Layer for Hybrid Perovskite/Si Tandem Devices

Elif Hüsam (Helmholtz-Zentrum Berlin)

We studied metal halide perovskites (HaPs) used as photoactive absorber layers in tandem solar cells and their buried interface with an evaporated C_{60} electron transport layer (ETL). The effect of interface engineering via the inclusion of a PEIE interlayer was probed by HAXPES. We present the chemical and electronic properties of the C_{60} /HaP interface as a function of a PEIE interlayer.

66 Going operando: Testing Solid-State Anode-free Lithium-Metal Batteries

Zora Chalkley (Helmholtz-Zentrum Berlin)

In anode-free lithium (Li) metal batteries (AFLMBs), Li metal is plated on a current collector degrading the electrode/electrolyte interface forming intermediates that we propose to probe with operando hard x-ray photoelectron spectroscopy (HAXPES). The range of information obtainable is presented herein. The impact of this data analysis is demonstrated by comparison of solid polymer electrolytes.

68 Controlled Polymorphism by Elevated Temperature Ball Milling

Kevin Linberg (Bundesanstalt für Materialforschung und -prüfung)

Mechanochemistry provides polymorphs that are difficult to obtain by conventional solution-based methods. Based on the nicotinamide and pimelic acid cocrystal, we demonstrated that the ball size, frequency, and temperature are essential parameters. Our results indicate that fine-tuning the energy input during a mechanochemical reaction can provide control over polymorphism.

69 Multi X-ray method approach to study zinc diffusion from restorative materials into tooth tissue

Oleksandra Marushchenko (Helmholtz-Zentrum Berlin)

Over time, restorative materials can be the source of diffusion processes in our teeth. The aim of the study is to better understand the microchemistry of dentin and the chemical changes at the interface between dental restorations and dentin, using both laboratory equipment and synchrotron experiments such as X-ray fluorescence and X-ray absorption near edge spectroscopy (XANES) analysis.

70 Instantaneous structural response of halide perovskites under illumination revealed by in-situ X-ray diffraction

Götz Schuck (Helmholtz-Zentrum Berlin)

Experiments on mySpot have shown that halide perovskites, such as $MAPbI_3$, respond to illumination with an immediate structural change. Rapid, reversible and slower, irreversible effects overlap. Structural response varies. Tilting of $[PbX_6]$ octahedra can be observed, as well as changes in Pb-X bond lengths and direct changes in halide anisotropic displacement parameters.

71 Crystallization study of transition metal phosphates: Characterization of a non-classical crystallization pathway

Stephanos Karafiludis (Bundesanstalt für Materialforschung und -prüfung)

In this study, we elucidate the crystallization of transition metal phosphates following a non-classical crystallization pathway. By using in-situ pH, X-ray scattering and diffraction in combination with electron imaging and elemental analysis (ICP-MS, cryo-TEM, EDX-SEM), the complex interplay between amorphous intermediates and final crystalline phases can be characterized.

73 Hydroxide based High Entropy Metal Organic Framework for Oxygen Evolution Reaction

Arkendu Roy (Bundesanstalt für Materialforschung und -prüfung)

High entropy metal hydroxide organic frameworks (HE-MHOFs) are composed of high entropy hydroxide layer inside MOFs, resulting in a high degree of structural complexity and diversity than conventional MOFs. It exhibits outstanding performance towards oxygen evolution reaction (OER) comparable to benchmark catalysts like IrO_2 and platinum carbon.

74 In-situ tomography with HDR imaging for process optimization of ceramic multilayer systems

Mustapha Eddah (Bundesanstalt für Materialforschung und -prüfung)

This project aims to quantify the structure and defect formation in LTCC systems using novel in-situ measurement methodology. A high dynamic range (HDR) method is being developed that allows a combination of different tomograms, each with X-ray energies adapted to individual materials. A furnace integrated into BAMline allows the observation of structure formation of LTCCs.

74 a Failure Mechanisms Investigation by Means of in-situ Synchrotron Computed Tomography in Aluminum MMC-based Alloy Tailored for Additive Manufacturing

Tatiana Mishurova (Bundesanstalt für Materialforschung und -prüfung)

Manufacturing of high-performance aluminium alloys by Powder Bed Fusion - Laser Beam (PBF-LB) is challenging dur to difficulties in printability. One approach is the addition of reinforcement to the based powder, allowing tailoring composition and properties of a Metal Matrix Composite (MMC) by additive manufacturing.

75 Electronic structure of VT and SCO complexes

Rainer Fink (FAU Erlangen-Nürnberg)

We report on the electron spectroscopic analysis of Fe-based spin crossover complexes (SCOs) and valence tautomers (VTs). These “smart” molecular systems allow one to controlling the spin and oxidation state of coordinated metal ions as proven by NEXAFS and XPS studies performed at the HE-SGM beamline.

76 Surface-mediated Charge Transfer of Photogenerated Carriers in Diamond

Arsène Chemin (Helmholtz-Zentrum Berlin)

Despite a large bandgap of 5.5 eV, charge carriers in diamond can be excited by visible light due to the presence of surface states. These transitions are identified using a combination of X-ray and UV/Vis spectroscopic techniques, providing a new understanding of the sub-bandgap photocurrent observed with diamond electrodes, which could enable visible light-driven photoelectrochemical CO_2 and N_2 reduction.

77 Surface characterization of covalently functionalized carbon-based nanomaterials using comprehensive XP and NEXAFS spectroscopies

Joerg Radnik (Bundesanstalt für Materialforschung- und prüfung)

XPS and NEXAFS are combined to precisely study and quantify the covalent functionalization of single-walled carbon nanotubes and nanographene by nitrene [2+1]-cycloaddition, where the preservation of the aromaticity corresponding to the π-conjugated system is demonstrated and successful post-modification by synthetic peptide or mannose is presented.

78 Improved estimation of the transmission function with UNIFIT 2022

Joerg Radnik (Bundesanstalt für Materialforschung- und prüfung)

Next to the established reference materials Cu, Ag and Au for estimating the transmission function, ionic liquids can be used for at beamlines with variable excitation energies. Comparison between the measured and stoichiometric composition shows that a transmission function was determined which allows a reasonable quantification.

79 Unravelling the chitin-protein packing in arthropod cuticle as a function of humidity

Gargi Joshi (Technische Universität Dresden)

Arthropod cuticle, a composite of chitin nanofibril embedded in a hydrated protein matrix, is organized over several length scales. We investigate the hydration mechanism in the cuticle of a spider for oriented chitin fibers using real-time SAXS/WAXS measurements at set relative humidities. We correlate anisotropic micro-strains observed in-situ on the individual components - protein and chitin.

80 NEXAFS and XPS on HE-SGM for analysis of the vessel conditions and onset fo the 2D material synthesis

Eva Kovacevic (CNRS / Univeristé d'Orléans)

HE-SGM offers unique possibility to concentrate on carbon based materials. We analyzed the traces of impurities collected from different places in chambers used for RF plasma synthesis of 2D structures. Already the traces of impurities (could not be followed by regular laboratory diagnostics) showed crucial for the control of onset and quality of the synthesis (very important for technology transfer).

81 Phase transitions of dimolybdenum tetraacetate on Cu(111): NEXAFS and XPS study

Alexei Nefedov (Karlsuher Institut für Technologie)

Dimolybdenum tetraacetate adsorbed on metal single crystal surfaces shows a transition from an ordered upright standing configuration to a phase with a flat lying configuration upon cooling. XPS/NEXAFS experiments have demonstrated that a molecule coverage is also very important for this transition. It was also established that both thermodynamics and kinetics play a crucial role in this process.

82 Temperature dependent photoemission studies of lead halide perovskites

Maryam Sajedi (Helmholtz-Zentrum Berlin)

ARPES of lead halide perovskite (LHPs) has yet only shown cubic bands at room temperature although the system is orthorhombic below 360K. We show weak orthorhombic features at 300K which become very pronounced at low temperature. Performing temperature dependent x-ray diffraction (XRD) and comparing ARPES to calculations based on XRD, we draw conclusions about high efficiency of LHPs.

108 XAS measurements of tridentate spin-crossover molecules adsorbed on graphite

Jorge Torres (Freie Universität Berlin)

A spin-crossover molecule (SCM) is a compound that can change its spin state from a low-spin to a high-spin state by temperature, pressure, or light. In this work, submonolayers of the SCMs $[Fe\{(H_2B)(pz)(pypz)\}_2]$ and $[Fe(pypypyr)_2]$ were deposited on HOPG and measured by XAS at PM-2 VEKMAG. For the former SCM, a thermal switch could be observed at room temperature, but not for the latter.

109 Long-periodic spin textures in vector magnetic fields as seen by resonant elastic x-ray scattering at VEKMAG

Victor Ukleev (Helmholtz-Zentrum Berlin)

Resonant elastic small-angle soft x-ray scattering (REXS) is the unique tool to study long-periodic spin textures in noncentrosymmetric magnets with unprecedented reciprocal-space resolution. The vector-field installation VEKMAG at PM-2 allows to probe such spin spirals at cryogenic temperatures and vector magnetic fields providing unique parameters of spin Hamiltonian hitherto unavailable by other probes.

110 PEAXIS - A Versatile RIXS Endstation for Energy and Quantum Material

Deniz Wong (Helmholtz-Zentrum Berlin)

High resolution RIXS allows the investigation of lattice system through the electronic structure providing insights toward the dynamics and transport properties of quantum materials. Furthermore, one would be able to probe distinct oxygen product that contributes to redox reaction inherent to new generation cathodes in Alkali ion batteries. This leads to a better understanding of the mechanism involved.

111 3D-surface reconstruction of cellular cryo-soft X-ray microscopy tomograms using semi-supervised deep learning

Michael Dyhr (Freie Universität Berlin)

Using a machine-learning approach, we trained a neural network to accelerate the process of 3D-segmentation of cryo-SXT datasets of vitrified mammalian cells. Our network automatically recognizes membrane structures in new, comparable datasets within as little as 10 minutes processing time on a single modern GPU, hence dramatically increasing the speed of the time-consuming segmentation process.

112 Analysis pipeline for for Correlative XAS and TEM Imaging

Christoph Pratsch (Helmholtz Zentrum Berlin)

Catalytic materials are dynamic under working conditions and understanding the time evolution of the local composition and oxidation states for different particles in different gaseous environments is critical for optimizing catalysts. To this aim we developed an analysis pipeline for our correlative in situ high resolution X-ray absorption spectromicroscopy (XAS) and transmission electron microscopy setup.

114 Spectromicroscopy of nanoscale materials in the tender X-ray regime enabled by a high efficient multilayer-based grating monochromator

Stephan Werner (Helmholtz Zentrum Berlin)

We report on a novel monochromator setup based on a multilayer coated blazed plane grating and plane mirror that improves the photon flux in the tender X-ray photon energy range 1.5 - 5.0 keV by two-orders-of-magnitude enabling previously unattainable nanoscale NEXAFS spectromicroscopy studies for applications in energy technologies and microelectronics.

115 ReMade@ARI - a hub for materials research for the circular economy

Lakshmi Bhaskaran (Helmholtz-Zentrum Dresden-Rossendorf)

ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Research Infrastructures) is committed to the development of innovative and sustainable materials for the circular economy. The project provides scientists from academia and industry exploring the properties and structures of recyclable materials with coordinated access to more than 50 analytical research infrastructures across Europe.

116 DAta from PHoton and Neutron Experiments (DAPHNE4NFDI)

Jan-Dierk Grunwaldt (Karlsuher Institut für Technologie / KFS)

Data from experiments with photons and neutrons are very valuable, but in Germany alone they amount to 30 PB/year. This large amount of data is often user-specific, cannot be easily shared and the analysis can be tedious. The goal of DAPHNE4NFDI is to increase the efficiency and reusability of this data by improved data workflows, accessible data repositories and fast, sophisticated analysis tools.

117 XAS Reference Database under DAPHNE4NFDI

Jan-Dierk Grunwaldt (Karlsuher Institut für Technologie / KFS)

Under DAPHNE4NFDI, we have set up an XAS reference database including raw and processed data with an interface developed for uploading and evaluating the data. Initial steps include defining metadata fields of a XAS experiment and formulating quality criteria. The interface includes an upload of metadata to the Scientific Catalogue and of files via object storage, with automated query capabilities.

118 How Are We Making Matter Data FAIR?

Gerrit Günther (Helmholtz Zentrum Berlin)

One of the key missions of HMC is to support the Helmholtz community in producing data according to the FAIR principles. Here, we present concrete approaches of HMC Hub Matter to make data of the BESSY II Light Source FAIR, ranging from uses cases at beamlines over training of the instrument staff to policy review and information tools.

119 Quality assessment of marble from the archaeological site of Pistiros

Ioannis Siouris (Democritus University Thrace)

SR-XRD and XRF techniques were used to determine the structural parameters and elemental synthesis of ancient marbles and quarries reference samples. The correlation of the analyzed data led to the determination of the origin of the marbles and pointed to specific quarries of Thassos island in Greece.

120 Ni-Fe bimetallic alloy on CeO_2-ZrO_2-Sm_2O_3 as electrode for Intermediate Temperature Solid Oxide Electrolyzer Cells

María del Rosario Suarez Anzorena (Helmholtz Zentrum Berlin)

Solid Oxide Electrolyzer Cells enable the production of CO and/or H_2 fuels from the electrolysis of CO_2 and/or H_2O. Operando studies on model cells based on near-ambient pressure X-ray Photoelectron Spectroscopy and grazing incidence X-ray diffraction show that Ni-Fe/CeO_2-ZrO_2-Sm_2O_3 has a great electrochemical performance and is resistant to carbon deposition while maintaining a stable structure.

121 The active state of oxides during electrocatalysis

Marcel Risch (Helmholtz-Zentrum Berlin)

We will present recent highlights of our group regarding the elucidation of the active state of electrocatalysts for the oxygen evolution reaction during operation.

122 In situ spectroscopic and analytical techniques to monitor particle formation

Monica Distaso (FAU Erlangen-Nürnberg)

Understanding particle formation is fundamental to rational design of functional materials. During particle formation, several chemical-physical phenomena occur over a broad range of sizes and time-scales. Herein, the use of multiple and simultaneous in situ analytical and spectroscopic techniques to monitor the evolution of the reaction mixtures in real time will be outlined for various materials.

123 Strain mapping of metallic cultural heritage objects with synchrotron microbeams

Alexander Schökel (Deutsches Elektronen-Synchrotron / DESY)

We present a proof of principle of radiographic strain mapping to retrieve markings in metallic objects. The strain patterns can be analyzed by Whole Powder Pattern Fitting, Rietveld refinement or even decorrelated by Principal Component Analysis of the integrated raw data to retrieve the erased hallmarks.

124 SyncLab – synergies offered by combined laboratory and synchrotron experiments

Ioanna Mantouvalou (Helmholtz-Zentrum Berlin / SyncLab)

The combination of laboratory and synchrotron experiments enables optimized beamtimes as well as the optimal use of instrumentation. We present case studies where these synergies are demonstrated with examples from biology, archeometry and photocatalysis.

125 Ultrafast wettability alteration: The decisive moments of adsorption on supported particles

Christian Weigelt (Universität Ulm)

The detection of intermediate species during photoinduced surface chemical reactions and the ability to correlate their ultrafast dynamics with the morphology and electronic structure of the surface is crucial to fully understand photoinduced or photocatalytic reactions. Prospective research directions aim at the investigation of catalytic water splitting facilitated by supported manganese oxide clusters.

126 The Femtoslicing Facility at BESSY II

Christian Schuessler-Langeheine (Helmholtz-Zentrum Berlin)

The Femtoslicing Facility at BESSY II provides 100-fs-short soft X-ray pulses with variable polarization plus a dedicated environment for ultrafast spin dynamics studies. For 2024 we plan the opening of a second beamline branch for experiments with higher energy resolution. The poster informs about recent and ongoing developments at the facility and gives an overview of recent scientific achievements.

129 Soft-XAS observation during CVD-Growth of oxides films: New Setup at UE56/1-SGM for studies at moderate pressure

Stefan Cramm (Forschungszentrum Jülich)

The structure of CVD grown films depend on the precursor gas pressure, growth temperature and, as recently observed, also on a magnetic field applied during growth. Detailed understanding e.g. of the latter mechanism is still missing. We built a setup to record absorption spectra during the growth and even gas phase absorption. First results on the growth kinetics of TiO_2 films from TTIP precursor are shown.

132 Structural properties of silver sulfide-reduced graphene oxide nanocomposite

Robert Ngure (Egerton University)

This paper reports the structural analysis of silver sulfide-reduced graphene oxide (Ag_2S-rGO) nanocomposite synthesized by chemical reduction method. SEM confirmed the formation of the nanocomposite by showing that rGO sheets were intercalated in Ag_2S nanoparticles and that Ag_2S had the shape of nanowires. X-ray diffraction revealed a d spacing ranging between 1.0 Å and 5.2 Å.

133 Morphological features and electrical properties of hollow SnO_2 for room temperature CO sensing

Bridget Mutuma (University of Nairobi)

This study highlights the synthesis of hollow SnO_2 nanostructures and their physicochemical properties. Hollow SnO_2 structures were utilized in the sensing of CO at room temperature and the sensor response was found to be six times higher than that of the solid SnO_2. This study indicated that the hollow SnO_2 obtained from a SiO_2 core-shell template has the potential to become a viable sensor material for CO.

145 High-valent intermediates observed in a Cu-based OER electrocatalyst by operando x-ray absorption spectroscopy

Raul Garcia-Diez (Helmholtz-Zentrum Berlin)

Copper as a promising candidate for alkaline water splitting, where high-valent Cu species are frequently proposed as key intermediates. This work benefits of the high chemical sensitivity of soft x-ray absorption spectroscopy to reveal the long-sought after high-valent Cu complex under operating conditions at the Cu L2,3-edge on an electrodeposited thin film of copper.

147 Unravelling the Effect of Pt isolation on shallow d-states of Gallium-Platinum Alloys

Tzung-En Hsieh (Helmholtz-Zentrum Berlin)

The properties of in-system prepared SiOx-supported GaPt alloys is examined by energy-dependent PES exploiting EMIL's two-color beamline. Pt isolation results in a narrowing and shift of the Pt 5d-derived band. Liquefaction, oxidation, and reduction of GaPt alloys with 1 at % Pt induces a surface enrichment of Pt and the formation of new phases, presumably representing the active catalyst surface.

148 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)

MXenes are a promising candidate for use in energy storage applications due to their high capacitance. Here, we monitor the chemical bonding of V_2CT_x MXene electrodes during cycling using operando X-ray absorption spectroscopy. Measurements at the V K-edge reveal changes of MXene surface chemistry.

149 Insights into the Electrolyte Lifecycle of High-Temperature Polymer Electrolyte Membrane Fuel Cells: Oxidation Behaviour of H_3PO_3 by in situ tender x-ray spectroscopies

Romualdus Enggar Wibowo (Helmholtz-Zentrum Berlin)

Recent studies suggest a possible conversion of H_3PO_4 to H_3PO_3 during the operation of HT-PEMFCs, which might poison Pt catalysts. In this work, we provide insights into the oxidation behaviour of aqueous H_3PO_3 on a Pt surface under conditions relevant to HT-PEMFCs operation, by a combination of in situ "Dip-and-pull" AP-HAXPES and P K edge XANES.

150 Deposition Sequence Matters: Differences in Model Ga-Pt SCALMS

Michael Moritz (FAU Erlangen-Nürnberg)

Catalysis on liquid metal alloys (SCALMS) is a new field in catalysis with striking potential. For developing this new concept, controlling the synthesis of these compounds is important. Here, model particles of Ga and Pt are prepared by PVD with different deposition orders and analyzed with XPS and TEM. The two particle systems show different properties, being highly relevant for future experiments.

151 Sulfur poisoning of PtGa SCALMS model systems

Christoph Wichmann (FAU Erlangen-Nürnberg)

The poisoning of SCALMS model systems by sulfur impurities was studied using XPS under UHV and near-ambient conditions. Formation of a Ga-sulfide layer was observed, where the incorporation of Pt is suggested. Formation of Pt-sulfides is not seen. For higher temperatures, dissolution of Ga-sulfides into the liquid metallic Ga-matrix is observed. The results suggest poisoning resistance in SCALMS catalysts.

152 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 provided are highly relevant in many research fields.

153 LiXEdrom: an experimental station dedicated to chemical investigation at BESSY II, utilizing XAS and RIXS

Ronny Golnak (Helmholtz-Zentrum Berlin)

The LiXEdrom is an experimental spectrometer dedicated to study liquid samples and solid-liquid interfaces with soft X-rays. The applicable methods are X-ray absorption (XAS) and resonant inelastic X-ray scattering (RIXS) which are powerful tools to investigate materials on an element selective level with respect to their atomic and electronic structure.

154 Photoelectron Spectroscopy from a Liquid Flatjet

Dominik Stemer (Fritz-Haber-Institut der Max-Planck-Gesellschaft)

We present the results of recent photoelectron spectroscopy experiments conducted at BESSY II using a liquid flatjet (FJ). Formed by the impingement of two cylindrical microjets, liquid (FJs) provide flexible experimental templates enabling unique liquid-phase experiments that would not be possible using single cylindrical liquid jets.

157 Tin-based phases engineering on planar and nanostructured silicon surfaces

Vladimir Sivakov (Leibniz Institute of Photonic Technology)

The electronic and atomic structure of the obtained Sn-based interfaces as promising anode for high-performance Li-ion batteries, or optical glasses or PCM for thermal energy storage, on the planar and in nanostructured Si surfaces, was investigated by NEXAFS and XPS using synchrotron radiation facilities at Diamond and BESSY II.

158 Epitaxial growth of hexagonal boron–nitrogen–carbon (h-BNC) monolayer on different substrate materials

Alaa Mohammed Idris Bakhit (Donostia International Physics Center)

We studied the epitaxial growth and electronic properties of a hybrid h-BNC monolayer on curved crystals c-Ni(111), c-Rh(557), and c-Pt(331). This h-BNC monolayer is a mixture of the two-dimensional layers of hexagonal boron nitride (hBN) and graphene (Gr). We observed that the catalytic activity for epitaxial growth is strongly dependent on the substrate material, growth temperature, and step density.

159 Photoelectron spectroscopy of van der Waals MPX3 compounds (M: Fe, Ni; X: S, Se)

Yuriy Dedkov (Shanghai University)

Here, by means of electron spectroscopy methods (NEXAFS and resonant photoelectron spectroscopy) in combination with density functional theory calculations and intensive structural studies we investigate the electronic structure of a new layered van der Waals MPX3 materials (M: Fe, Ni; X: S, Se).

161 Nanoscale infrared spectroscopy at the IRIS Beamline

Alexander Veber (Humboldt Universität zu Berlin)

Recently nanospectroscopy end station has broadened the palette of the infrared techniques available at the IRIS beamline. The new technique allows to collect IR spectra and perform chemical imaging at spatial scales down to 20 nm. Here we show the characteristics of the end station and demonstrate its capabilities for the investigation of complex biological and synthesized composite materials at nanoscales.

162 Nanoscale-spectroscopy and Imaging of Protein Aggregates

Antonia Intze (Sapienza University of Rome)

Self-assembly of proteins into nanoscale aggregates and finally into fibril microbundles is linked to neurodegeneration. Here, we study the aggregation pathway of alpha-synuclein protein by using the IR micro-spectroscopy and AFM-assisted IR nano-spectroscopy (AFM-IR) technique. The use of high lateral resolution IR micro-spectroscopy with synchrotron radiation can provide a benchmark for AFM-IR experiments.

163 Light-induced conformational changes of transmembrane proteins probed by difference IR microspectroscopy with Synchrotron radiation and nanospectroscopy

Raffaella Polito (Sapienza University of Rome)

We apply mid-Infrared (mid-IR) microspectroscopy performed with Synchrotron radiation to investigate the conformational changes of light-sensitive transmembrane proteins widely used in bioelectronic devices and optogenetic applications. The results are a good benchmark for our experiments of mid-IR nanospectroscopy based on the use of an atomic force microscope.

169 Bimetallic Ni-based catalysts for urea oxidation reaction: the effect of Co and Fe on the relationships between the structure and the activity of the catalyst

Viktoriia Zemtsova (Université de Strasbourg / ECPM)

Ni is a promising and the most studied catalyst for urea oxidation reaction. In this project we propose to investigate the dynamic changes of the structure and the oxidation state of Ni, Ni(Fe) and Ni(Co) nanoparticles using operando XAS to advance the understanding of the nature of active sites in the urea oxidation reaction (UOR).

170 Complementary X-ray techniques reveal hidden details in dental materials

Leona Bauer (Technische Universität Berlin)

The combination of synchrotron radiography and laboratory CμXRF, XAS and μXCT measurements enables the structural and elemental investigation of a sample. Using information from all these methods, an algorithm has been developed for the absorption correction of CμXRF data obtained at the interzone of dental materials, paving the way for a 3D quantitative elemental analysis of heterogeneous samples.

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

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, which is under development at BAMline and dedicated for characterization of porous solids under working conditions.

172 Visualization of Deep discharge mechanism using operando XCT

Shahabeddin Dayani (Bundesanstalt für Materialforschung und -prüfung)

Thanks to their high brilliance, synchrotron beam facilitates us to do a full Computed Tomography in a short time. This enables us to measure batteries while being cycled with a reasonable time resolution to record morphological changes. In this presentation we illustrate how one can utilize this ability to investigate abuse mechanisms on an actual commercially available lithium-ion battery from cell level.

173 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 behavior.

174 BAMline – A real-life samples materials research beamline

Ana Guilherme Buzanich (Bundesanstalt für Materialforschung und -prüfung)

We provide an overview of analytical methods and sample environments of the BAMline that fall into the X-ray absorption and X-ray fluorescence spectroscopy categories (XAS, XRF). With own synthesis methods, processes and equipment we provide real-time optimization of material properties and performance for various applications such as energy storage, catalysis, and corrosion resistance.

175 EXAFS elucidating local structure of amorphous heterogeneous catalysts in C-F-bond activation

Christian Heinekamp (Bundesanstalt für Materialforschung und -prüfung)

Amorphous materials play an important role in C-F bond activation but face the difficulty of limited available structural information by methods such as powder XRD and solid-state MAS NMR spectroscopy. Here, we present heterogeneous catalysts, active in C-F bond activation, where EXAFS allowed specifically elucidating the local structure, which would have not been possible elsewise.

176 Synchrotron X-Ray Tomography Techniques at BAMline

Henning Markötter (Bundesanstalt für Materialforschung und -Prüfung)

A recent upgrade of BAMline's major instruments expands its imaging capabilities: shorter scan acquisition times are now possible, in situ and operando studies can now be routinely performed, and different energy spectra can be easily set up. The double multilayer monochromator offers full flexibility by providing different energy spectra to optimize flux and energy resolution as desired.

193 Effektives und kalibrierbares hochauflösendes wellenlängendispersives Röntgenemissionsspektrometer für polarisationsabhängige Messungen im Spektralbereich weicher Röntgenstrahlung

Jan Weser (Physikalisch- Technische Bundesanstalt)

In der PTB wurde in Kooperation mit dem NIST ein neues wellenlängendispersives Spektrometer (WDS) entwickelt, welches für polarisationsabhängige Messungen zur Röntgenemissionsspektrometrie (XES) und zur resonanten inelastischen Röntgenstreuung (RIXS) im Photonenbereich von 80 eV bis 1100 eV ausgelegt wurde. Es soll zu einem besseren Verständnis der elektronischen Struktur verschiedenster Materialien dienen.

194 Reconstruction of TiO_2-HfO_2 gratings with scanning-free grazing emission X-ray fluorescence

Nils Wauschkuhn (Physikalisch-Technische Bundesanstalt)

The growing complexity of today's semiconductor-related nanostructures requires advanced metrology techniques. In this study, we demonstrate the capability of scanning-free grazing emission X-ray fluorescence (GEXRF) for two-dimensional nanostructures. TiO_2 gratings with different etching depths, coated with HfO_2, are characterized dimensionally and analytically using GEXRF.

195 Reconstruction of periodic nanostructures with grazing incidence X-ray fluorescence and influence of roughness effects

Vinh Truong (Physikalisch-Technische Bundesanstalt)

GIXRF measurements are non-destructive and element-specific with high sensitivity for nanostructured surfaces. For further development as a dimensional and analytical tool for nanometrology, it is essential to model the influence of roughness and other periodicity disturbances. First approximations of roughness effects have been simulated and presented in more detail.

196 Towards a laboratory-based reference-free X-ray fluorescence analysis

André Wählisch (Physikalisch-Technische Bundesanstalt)

A reliable XRF analysis can be achieved by utilizing precise knowledge of the spectral distribution of the excitation source. By using the calculable synchrotron radiation from a bending magnet, this work shows that a reference-free XRF approach can be implemented for polychromatic excitation conditions. The same principles may readily be transferred to similar X-ray sources, such as X-ray tubes.

197 Influence of model imperfections on shape reconstruction of nanostructures from grazing incidence X-ray fluorescence measurements

Kas Andrle (Physikalisch-Technische Bundesanstalt)

GIXRF measurements are used to reconstruct nanogratings. The fluorescence signal depends on the elemental composition and dimensional properties. A FEM-based Maxwell solver calculates the XSW field, allowing simulation and reconstruction of the data. The effect of model imperfections on the reconstruction is important to analyze, since simulations assume an ideal model.

198 Monitoring the Formation of Nickel-Poor and Nickel-Rich Oxide Cathode Materials for Lithium-Ion Batteries with Synchrotron Radiation

Ying Bixian (Universität Münster)

The syntheses of Ni-poor (NCM111) and Ni-rich (NCM811) lithium transition-metal oxides are investigated using in situ synchrotron powder diffraction and near-edge X-ray absorption fine structure spectroscopy. he synthesis of NCM811 incorporates an intermediate phase with a rock salt-type structure, whereas NCM111 maintains a layered structure throughout the entire synthesis process.

199 New micro focus beamline for Tender X-rays in the PTB Laboratory at BESSY II

Matthias Müller (Physikalisch-Technische Bundesanstalt)

PTB's new beamline at BESSY II started commissioning. The beamline provides dipole radiation in the tender x-ray energy range from 1.5 keV to 8.0 keV using a combined multilayer-coated PGM and DCM. The beam is focused to the experiment to a spot size of 5 µm to 40 µm. The beamline is designed for metrology and x-ray spectrometry measurements requiring a high spectral purity and beam stability.

200 Parametric optimization routines for a calibrated, double full cylinder von Hamos spectrometer

Kai Schüler (Physikalisch-Technische Bundesanstalt)

The parametric optimization routines minimize the broadening of emission lines and the loss of fluorescence photons, which are induced by any misplacement of the optical components, and enhance the alignment reliability, by quantifying its quality and ensuring its reproducibility. With the routines, the alignment of the spectrometer is no longer empirical, but subject to a reproducible optimization procedure.

200 a Absolute number concentration measurements of nanoparticles by small-angle X-ray scattering (SAXS)

Robin Schürmann (Physikalisch-Technische Bundesanstalt)

Small-angle X-ray scattering is a powerful tool to determine the size, shape and concentration of nanoparticles. To calculate number concentrations, absolute measurements of the scattering intensity in terms of SI-units are necessary, which require accurate knowledge of all experimental parameters and the electron density of the particles that must be determined by complementary techniques.

200 b 2 Dimensional X-ray Scattering Patterns of Magnetic Nanoparticles in a Magnetic Field

Dieter Skroblin (Physikalisch-Technische Bundesanstalt)

Magnetic anisotropy is the reason why magnetic nanoparticles tend to orient themselves in a magnetic field. As a result, the X-ray scattering patterns of such oriented systems collected on 2D area detectors have a strong directionality. We present small-angle X-ray data of particles measured in a magnetic sample environment and show how to calculate the corresponding oriented form and structure factors.

200 c Modulated grazing exit fluorescence radiation from nanostructured surfaces under grazing incidence

Victor Soltwisch (Physikalisch-Technische Bundesanstalt)

The diffuse scattering often observed on nanostructured surfaces with GISAXS hides more information than is apparent at first glance. Roughness models this diffuse scattering and allows, for example, conclusions to be drawn about line edge roughness in gratings. At the same time, modern area detectors can also pick up fluorescence signals, which are usually superimposed on the elastic scattering.

CR a Characterization of different battery materials using X-ray spectrometry

Lena Mathies (Physikalisch-Technische Bundesanstalt)

At two PTB beam lines different battery materials were investigated by means of X-ray spectrometry. PTB can quantify the mass deposition of selected elements to investigate battery degradation processes or material decomposition after cycling. Initial measurements to assess the challenges for operando battery experiments were performed and the proof of concept of Na battery operando experiment was confirmed.

CR b Uncertainty of Dimensional Nanoscale Grating Reconstruction

Leonhard Lohr (Physikalisch-Technische Bundesanstalt)

Shape reconstruction of nanoscale gratings is important for the semiconductor industry. Scatterometry using synchrotron radiation and finite element simulations can accurately determine a grating shape. Markov chain Monte Carlo sampling provides uncertainty estimates. Combining soft X-ray scattering and fluorescence, as shown in a recent experimental study, could increase reconstruction accuracy.

CR c Small-Angle X-ray Scattering (SAXS): Characterization of arbitrarily shaped nanoparticles using Debye's scattering formula

Jerome Deumer (Physikalisch-Technische Bundesanstalt)

We propose a user-friendly approach to calculate scattering profiles of complex shaped nanoparticles for SAXS using the Debye equation. This equation allows to compute the SAXS pattern of an ensemble of virtual scattering points. First, a randomly distributed point cloud of the aimed particle shape is generated. Then, Debye's formula is applied to it to calculate the SAXS pattern of a single particle.

CR d Optical constants and their influence on the reconstruction of periodic nano-gratings using EUV scatterometry

Richard Ciesielski (Physikalisch-Technische Bundesanstalt)

We present elastic scattering data from complex, periodic nanostructures. These scatterometry measurements can be used for geometrical reconstruction of feature sizes in the nanometer range. Here, the precise knowledge of the optical constants of the materials in question is essential. For that reason, PTB works on a freely accessible database of optical constants.

CR 1 Use of a Timepix 3 detector in X-PEEM

Florian Kronast (Helmholtz-Zentrum Berlin)

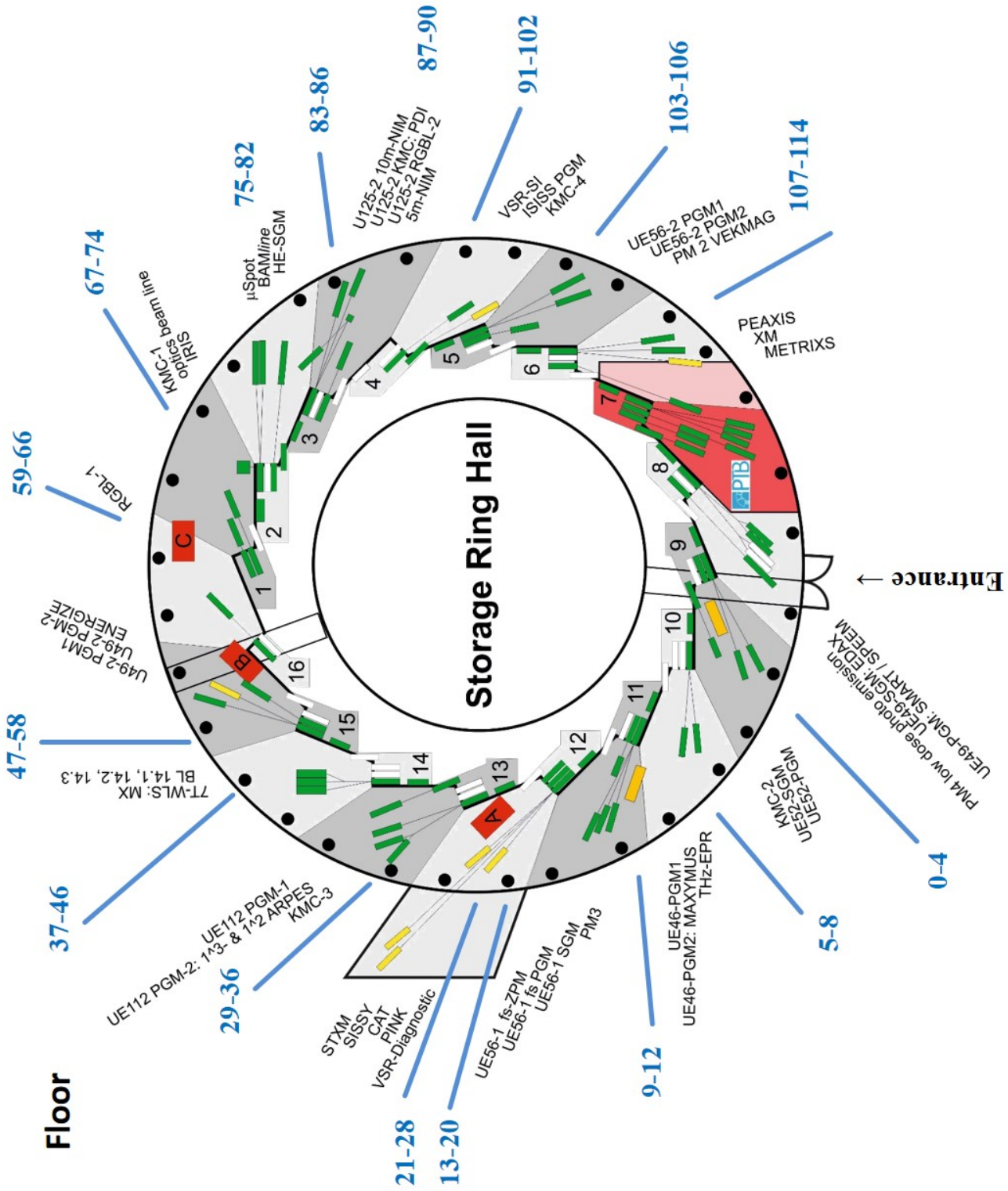
PEEM with a Timepix3 detector, a time-resolved direct electron detector with 512 x 512 pixels (quad configuration) and an intrinsic time resolution of 1.6 ns, as well as two additional TDC channels with a time resolution of 256ps. Here we will present our first experiences and results, the achieved time resolution, but also other advantages like improved quantum efficiency and no crosstalk between pixels.

CR 2 X-ray imaging of 2D materials: magnetic domains and time-resolved experiment

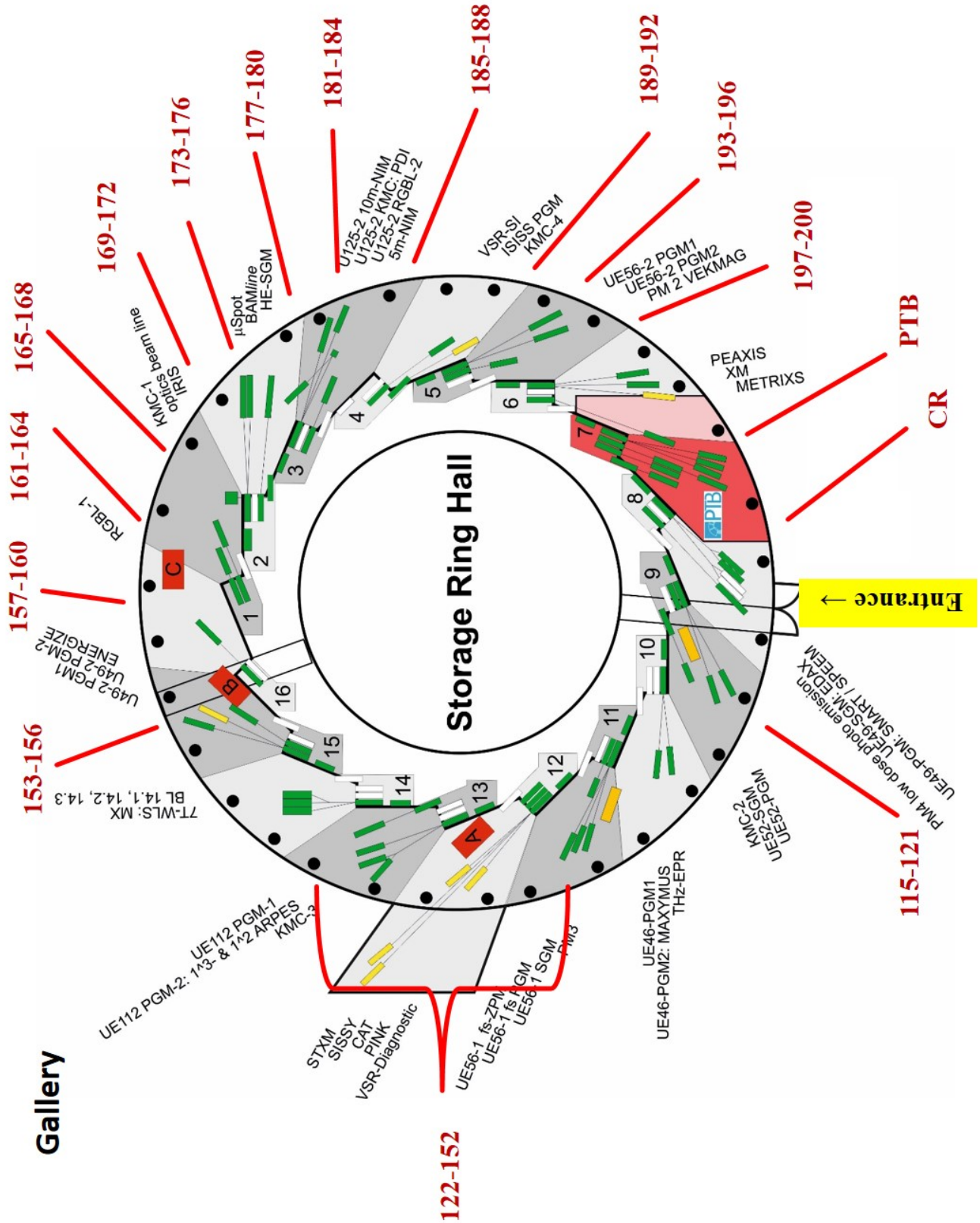
Alevtina Smekhova (Helmholtz-Zentrum Berlin)

We employed XPEEM imaging to study macroscopic flakes of atomically thin heterostructures based on the van der Waals Fe_5GeTe_2 ferromagnet and prepared by exfoliation in inert atmosphere. The magnetic domains observed at temperatures around 40 K reveal a pronounced thickness dependence, whereas fs laser pulses were used to optically excite the 2D structure under investigation.

Floor Plan Poster Session - Ground Floor



Floor Plan Poster Session - Gallery / First Floor



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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.

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Vendor Exhibition

Thursday, 22 June from 09:00 to 17:00

Friday, 23 June from 08:30 to 14:30

WISTA Conference Center

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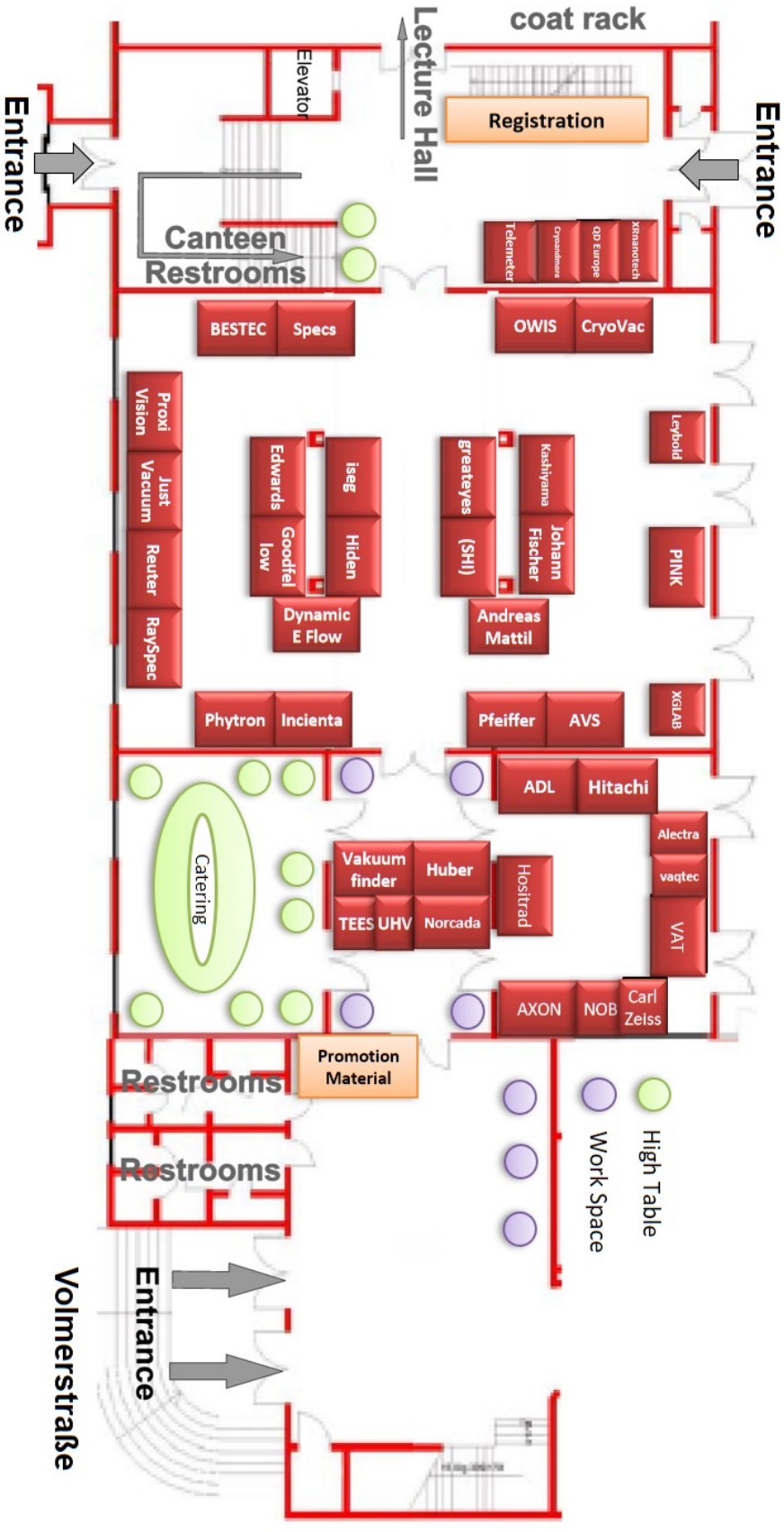
Floor Plan - Vendor Exhibition



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Campus Map Berlin-Adlershof

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

WISTA Conference Center
Rudower Chaussee 17
12498 Berlin

① Train station Adlershof

② WISTA Conference Center
Registration
Bunsen-Hall
Vendor Exhibition

③ BESSY II Experimental Hall
Poster Session

④ Dorint Hotel Adlershof

⑤ Airporthotel Adlershof

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HZB BESSY II Light Source

Call for Proposals

HZB kindly invites you to submit BESSY II proposals for the next allocation period from January 2024 to July 2024.

BESSY II beamtime applications may only submitted via the general access tool GATE

http://hz-b.de/gate

DEADLINE
1 Sept. 2023