HZB BESSY II Light Source

14th BESSY@HZB User Meeting

December 8th, 2022

INVITED SPEAKER

Public Lecture	Seth R. Marder (CU-Boulder/NREL, US)
Energy Conversion	Jan Niklas Hausmann (TU Berlin, DE)
Energy Storage	Sven Hampel (TU Clausthal, DE)
Information Technology	Lourdes Marcano (UPV/EHU, ES)
Life Science & Health	Nils Schuth (Cinvestav, MX)
Life Science & Health@MX	Friederike Füsser (Uni Münster, DE)
Matter & Material	Mayara da Silva Santos (HZB, DE)
4000th Protein Structure@MX	Christian Meyners (TU Darmstadt, DE)

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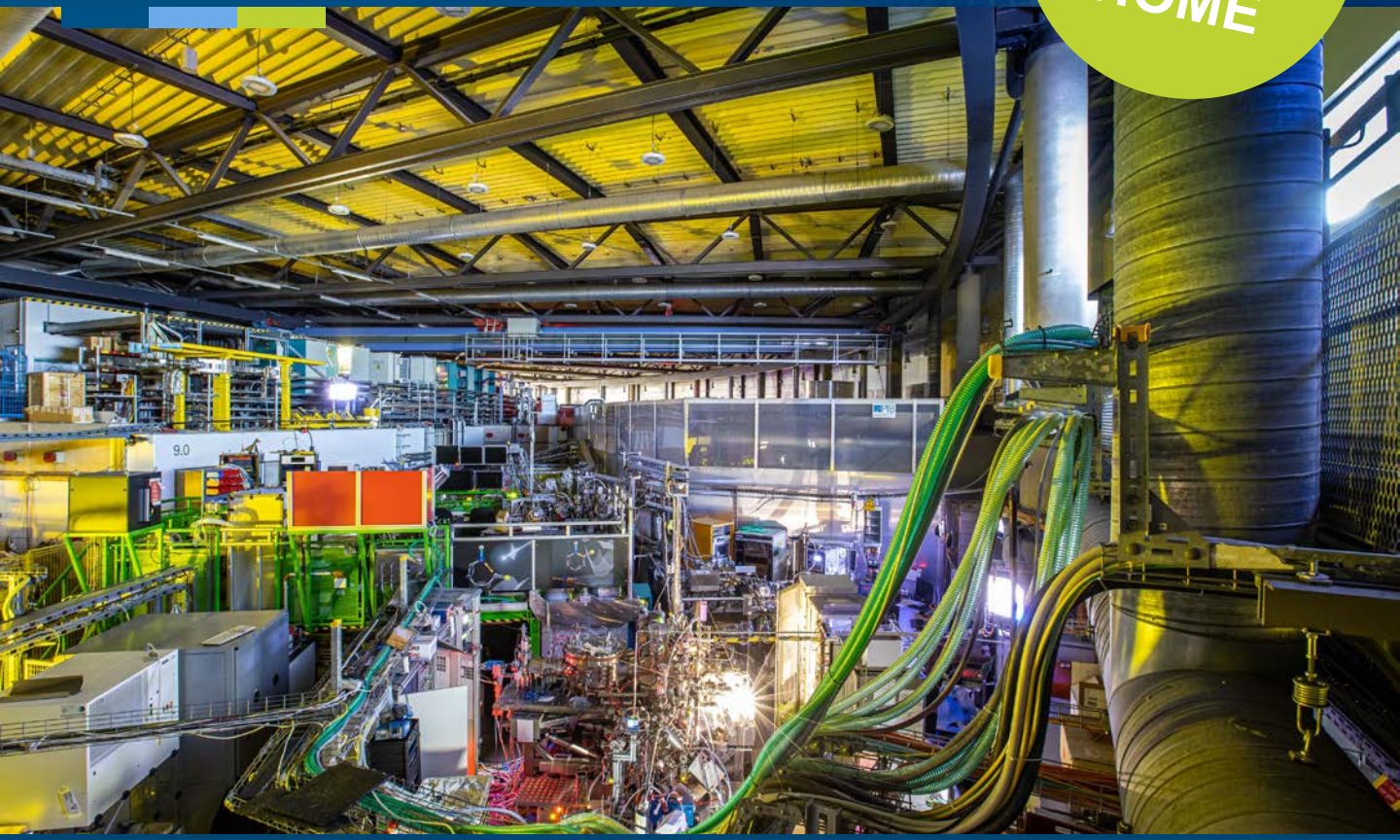

Poster Session Poster Slam Vendor Exhibition

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WELCOME

Dear Users and Friends,

Welcome to the 14th BESSY@HZB User Meeting 2022.

This year - due to the ongoing pandemic and for the third time in a row - the BESSY@HZB User Meeting takes place as a virtual 1-day meeting, but we are very pleased to announce that we will break with our long-standing tradition of Christmas meetings: The User Meeting 2023 will be held in summer; live and on-site in Berlin-Adlershof on June 22nd and 23rd. No gingerbread and scent of fir, but ice cream and sunshine!

Next year's User Meeting in summer also offers a great opportunity to celebrate two anniversaries. 40 years of research with synchrotron light in Berlin and the 25th anniversary of BESSY II: in 1982, the first electron storage ring BESSY (Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung) went into operation in Berlin-Wilmersdorf and the successor facility BESSY II in Berlin-Adlershof produced its first light beam in 1998. For decades, science in Berlin has been an important driver of innovation and progress, and many discoveries - from fundamental insights to marketable products - are results of research with synchrotron light.

Last summer, to ensure the long-term operation of BESSY II over the next decade, we went into a 14-week shutdown, the longest in BESSY II history. And even though no science took place, BESSY II was a magnet for visitors. We were delighted to welcome the German Federal Minister for Education and Research Bettina Stark-Watzinger, Carl XVI. Gustaf the king of Sweden, high-ranking delegations from Singapore and Brazil, a lot of high school kids and students, and many interested visitors at the "Long Night of the Sciences 2022".

Amazing science returned in September when 400 experts from Germany and Europe met in Berlin to exchange knowledge and ideas at the SNI2022 (the German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities). The conference was organised by HZB in cooperation with the Komitee Forschung mit Synchrotronstrahlung (KFS), the Komitee Forschung mit Neutronen (KFN) and the Komitee Forschung mit Sonden und Ionenstrahlen (KFSI). Presentations covered the entire field from curiosity driven investigations of fundamental principles to application-oriented development of materials and devices. Highlighting the societal relevance of research at large scale facilities was also the topic of the public lecture.

International cooperation and science diplomacy are the basis for another very important project. A new experimental set-up has been opened at the X-ray source SESAME in Jordan: HESEB, the Helmholtz-SESAME Beamline, designed by five research centres of the Helmholtz Association. Experts from HZB designed and built the undulator that generates the appropriate light spectrum for the HESEB beamline. They used refurbished components from the UE56-2 undulator combined with a new magnet array assembled, measured and tuned in Berlin over the last two years.

WELCOME

The past year also brought us sad and reflective moments. It was with great dismay that we and the entire Alliance of German Science Organisations have followed Russia's military attack on Ukraine launched in February. We all regard the Russian invasion as an attack on the fundamental values of freedom, democracy and self-determination, which in turn provides the basis for academic freedom and opportunities for academic cooperation. We have since long maintained diverse and productive academic collaborations with our partners in Ukraine and they have our full solidarity and support.

This war affects all of us and forces us and in particular, a large-scale research facility like BESSY II, to reduce our energy consumption and increase our energy self-sufficiency even more than before. We have received many requests from concerned users if there are any considerations to shut down BESSY II due to its high energy consumption. Research at BESSY II is the basis for a secure, sustainable energy supply of the future and must continue. According to the current state of planning, we assume that we will be able to operate BESSY II without interruptions in the winter of 2022/23.

Sustainability and environmental protection are also important issues in HZB's latest international cooperation project CARE-O-SENE. This project brings together seven major German and South African partners to develop optimised catalysts for the production of green kerosene. CARE-O-SENE will play a key role in sustainably transforming industries such as aviation. The goal is to make the production of green kerosene as a fuel alternative economically more attractive.

The CARE-O-SENE project illustrates very well HZB's activities in the field of energy conversion and energy storage. Life science & health, information technologies and matter & materials, the other major scientific topics are also represented in this year's programme and will again underline the broad variety of scientific fields addressed by the experiments performed by you at the HZB facilities.

This year's Public Lecture "Thoughts About the Right Here, Right Now Global Climate Summit" which Seth Marder, director of the Renewable and Sustainable Energy Institute (CU-Boulder and NREL) kindly accepted to present, will certainly be the highlight of the programme.

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

Enjoy the meeting!

Sincerely,

Prof. Dr. Bernd Rech

Scientific Director

PROGRAMME

14th BESSY@HZB User Meeting on Thursday, 8th of December 2022		
08:00 - 09:00	Registration & Lobby Talk	60 Min.
08:15 - 09:00	Networking Carousel - Match Making Event	45 Min.
09:00 - 10:20	**Synchrotron Session (Chair: Christian Jung)**	**80 Min.**
09:00 - 09:10	Bernd Rech - Welcome to the User Meeting 2022	10 Min.
09:10 - 09:30	Antje Vollmer - News from BESSY II and BESSY III	20 Min.
09:30 - 09:50	Markus Ries - Operation and Development of BESSY II and MLS	20 Min.
09:50 - 10:00	Jan-Dierk Grunwaldt (KIT, DE) - KFS	10 Min.
10:00 - 10:10	Cormac McGuinness (TCD, IR) - The European Synchrotron and FEL User Orgainsation (ESUO) - Working on behalf of users	10 Min.
10:10 - 10:20	Silvana Westbury (Diamond, UK) - lightsources.org	10 Min
10:20 - 11:00	Break: Vendor Exhibition & Poster Exhibition & Lobby Talk	40 Min.
11:00 - 12:00	**Scientific Lectures - Part I (Chair: Vicente Zamudio-Bayer)**	**60 Min.**
11:00 - 11:20	Energy Conversion - Jan Niklas Hausmann (TUB, DE) The Effect of Precatalysts and Reconstruction Conditions on the Oxygen Evolution Reaction	20 Min.
11:20 - 11:40	Energy Storage - Sven Hampel (TU Clausthal, DE) Vanadium speciation in polymer electrolyte membranes used in vanadium redox flow batteries	20 Min.
11:40 - 12:00	Matter & Material - Mayara da Silva Santos (HZB, DE) Identification of reactive metal-oxygen species in the gas phase *via* soft X-ray spectroscopy	20 Min.
12:00 - 13:00	Break: Vendor Exhibition & Poster Exhibition & Lobby Talk	60 Min.
12:30 - 13:00	Networking Carousel - Match Making Event	30 Min.
13:00 - 14:20	**Scientific Lectures - Part II (Chair: Frank Lennartz)**	**80 Min.**
13:00 - 13:20	The 4000th protein structure at MX - Christian Meyners (TU Darmstadt, DE) Structure-based drug discovery for FKBP51 – targeting depression, chronic pain and diabetes	20 Min.
13:20 - 13:40	Life Science & Health at MX - Friederike Füsser (Uni Münster, DE) Fragment-based drug design for the development of new antituberculosis drugs	20 Min.
13:40 - 14:00	Information Technology - Lourdes Marcano (UPV/EHU, ES) Quantifying the magnetic anisotropy of magnetic nanoparticles in biological vehicles	20 Min.
14:00 - 14:20	Life Science & Health - Nils Schuth (CINVESTAV, MX) *In vivo* detection of zinc-storing compounds in Drosophila utilizing X-ray absorption spectroscopy	20 Min.
14:20 - 15:00	Break: Vendor Exhibition & Poster Exhibition & Lobby Talk	40 Min.
15:00 - 16:00	**Poster Slam (Chair: Roland Müller)**	**60 Min.**
16:00 - 17:00	**Poster Session - Live chats with poster presenters**	**60 Min.**
17:00 - 18:00	**Public Lecture (Chair: Norbert Koch)** **Seth R. Marder: Thoughts About the Right Here, Right Now Global Climate Summit**	**60 Min.**

ABSTRACTS OF THE SCIENTIFIC LECTURES

SCIENTIFIC TOPICS

Energy Conversion

Energy Storage

Matter & Material

Life Science & Health

Information Technology

Public Lecture

The Effect of Precatalysts and Reconstruction Conditions on the Oxygen Evolution Reaction

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The oxygen evolution reaction (OER) is the most likely reaction to supply electrons and protons for future green fuel and chemical formation and thus many materials have been studied for their suitability as OER (pre)catalysts. However, *in-situ* and post-catalytic studies have shown that the harsh OER conditions alter the electrode materials causing a reconstruction to mainly transition metal oxyhydroxides in alkaline and near-neutral electrolyte. As this reconstructed phase is the real catalyst, its atomic structure and physical properties must be precisely known. These properties will be affected by the precatalyst and the reconstruction conditions like the product of a chemical reaction is affected by the substrate and reaction conditions. For the elucidation of such reconstruction processes, spectroscopic (*in-situ*) methods combined with new, meaningful precursors are required.

Herein, investigations on the reconstruction of several precatalysts such as borophosphates,[1] selenites,[2] and elemental metal foam[3] are presented. These reconstructions were analysed by *in situ* Raman and X-ray absorption spectroscopy together with state-of-the-art post-mortem characterisation techniques. In an effort to connect this data, we propose ideas relating the precatalyst structure with the one of the formed oxyhydroxides and their catalytic properties. Moreover, as mentioned, also the reconstruction conditions affect the specific nature of the formed oxyhydroxide. Considering this, we show that from the same precatalyst, catalysts with entirely different structural and electrocatalytic properties can be obtained by only changing the electrochemical reconstruction conditions (potential, pH, electrolyte composition...).

References:

[1]Adv. Mat. 207494 (2022)

[2]Energy. Environ. Sci. 13, 3607 (2020)

[3]Adv. Energy Mat. 12, 2202098 (2022)

Vanadium speciation in polymer electrolyte membranes used in vanadium redox flow batteries

S. Hampel[1], C. Lutz[1], X. Ke[1], M. Stehle[1], S. Beuermann[1], T. Lemmermann[1], T. Turek[1], U. Kunz[1], M. Becker[1], A. Guilherme Buzanich[2], M. Radtke[2], J. Garrevoet[3], G. Falkenberg[3], U. E. A. Fittschen[1]

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Vanadium redox flow batteries (VFB) are promising candidates for stationary energy storage. They consist of two half cells, which are connected to the electrolyte containers. Both half cells are separated through a polymer electrolyte membrane (PEM) which usually consists of perfluorosulfonic acid ionomers (*e.g.* Nafion™). Nafion™ offers good chemical and mechanical stability but exhibits a poor ion selectivity. Besides protons, water and vanadium species are transported through the membrane. This strongly contributes to capacity fade, and often is referred as 'cross over effect'. A good knowledge of the processes inside the membrane is crucial to improve materials and theoretical knowledge. Previous theoretical models, *e.g.*, consider only the transport of the individual vanadium species, but not reactions within the PEM.

Bulk vanadium speciation in PEMs in the laboratory is often accomplished with UV-VIS absorption spectroscopy and lately also by X-Ray absorption near edge structure spectroscopy (XANES) [1,2]. Results obtained from these experiments formed the basis for spatially resolved XANES at BESSY II and PETRA III (DESY). At the BAM*line* (BESSY II) we proved the reaction of V(III) and V(V) to V(IV) inside Nafion™ for the first time [3]. Radiation damage was observed during a long time X-Ray exposure at the BAM*line* leading to oxidation of V(III) to V(IV) [3]. This needs to be reduced for measurements with higher flux density performed at P06. The resolution of 0.5 µm was needed to record vanadium species profiles *through-plane* of the PEM. Therefore, a procedure was established at P06 (Petra III) for using *through-plane* diffusion cells and a cryo stream for minimal oxidation of the sensitive vanadium species [4].

Besides Nafion™, novel grafted-PEM based on poly(1,1-difluoroethylene) (PVDF) were probed. They are expected to provide better ion selectivity while maintaining good chemical and mechanical stability to replace the expensive Nafion™ in the future.

References:

[1] Membranes 11, 576 (2021)

[2] Powder Diffr., 1 (2020)

[3] J. Power Sources 483, 229176 (2021)

[4] J. Synchrotron Rad. 28, 1865 (2021)

Identification of reactive metal-oxygen species in the gas phase *via* soft X-ray spectroscopy

M. da S. Santos[1,2], M. Flach[1,2], O. S. Ablyasova[1,2], M. Timm[2], B. v. Issendorff[1], K. Hirsch[2], V. Zamudio-Bayer[2], T. Stüker[3], S. Riedel[3], and J. T. Lau[1,2]

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Discovering compounds that present transition metals with unusual oxidation states or reactive oxygen species (superoxido, peroxido and oxygen centered radical) is of great scientific and technological interests, as they have key applications as oxidizing agents, catalysts, or reaction intermediates.

Here, we use X-ray absorption spectroscopy (XAS) at the oxygen K and metal L_3, M_3 or N_3 edges of $[MO_n]^+$ systems (M = transition metal, n = integer) to identify the spectroscopic signatures of oxygen ligands and assign the oxidation state of the metal. The $[MO_n]^+$ species are investigated in the gas phase and are produced by argon sputtering of a metal target in the presence of oxygen. The cationic species are mass selected and accumulated in an ion trap. X-ray absorption spectra are then recorded in partial ion yield mode. The experiments were performed at the Ion Trap station at the undulator beamline UE52-PGM at the Berlin synchrotron radiation facility BESSY II.

Cationic species containing reactive oxygen ligands, such as the ozonido $[Cu(O_3)]^+$, the oxygen centered radical $[RuO_4]^{+\bullet}$ and biradical $[ReO_4]^{+\bullet\bullet}$, and species containing high-valent transition metals such as the rhodium(VII) trioxido cation, $[RhO_3]^+$, are analyzed under controlled conditions in their electronic ground state inside the cryogenic ion trap. This method is here demonstrated to be an important tool to elucidate such highly reactive species, offering direct access to their electronic structure with element specific sensitivity.

References:

Phys. Chem. Chem. Phys. 13, 1925–1938 (2011)

Coord. Chem. Rev. 253, 606–624 (2009)

Angew. Chem. Int. Ed., e202207688 (2022)

Phys. Chem. Chem. Phys. 24, 3598–3610 (2022)

J. Phys. B: At., Mol. Opt. Phys. 42, 154029 (2009)

Structure-based drug discovery for FKBP51 – targeting depression, chronic pain and diabetes

Christian Meyners[1], Jorge A. Lerma Romero[1], Andreas, Christimann[1], Lisa M. Reinbold[1], Anna Charalampidou[1], Harald Kolmar[1], Felix Hausch[1]

1 Institute for Organic Chemistry and Biochemistry, Technical University of Darmstadt, Germany

Depression, chronic pain or obesity-associated diseases (e.g. diabetes) are servere and insufficiently treatable diseases which according to the WHO will be one of the biggest health issues by 2030. The FK506-binding protein 51 (FKBP51) regulates the signal transduction of steriod hormone receptors and has emerged as a promising drug target for these diseases. The 4000th protein structure from HZB BESSY released in the PDB shows the G64S variant of FKBP51 in complex with the highly selective ligand SAFit1[1]. Ligands of the SAFit-series are first-in-class compounds which are widely used as tool compounds for the pharmacological validation of FKBP51 in animal models. However, the selectivity and physiochemical properties of these ligands are not good enough yet and for the development of a clinical candidate novel FKBP51 selective compounds have to be identified. The selectivity of SAFit1 and other FKBP51 selective ligands is due to binding to a FKBP51 conformation with an altered binding site. This conformational rearrangement is highly disfavored in other FKBP proteins. Unfortunately, selective FKBP51 ligands are hard to identify by classic screening approaches since the binding active conformation with an open selectivity pocket is only populated to a very low extent. The aforementioned G64S variant of FKBP51 was identified by high throughput protein engineering and has a stabilized binding pocket. This variant binds serveral times stronger to FKBP51-selective ligands and by solving the structure of the G64S variant of FKBP51 in complex with SAFit1 we were able to show that this is indeed due to a stabilization of the selectivity pocket in the open conformation. This new FKBP51 variant will be used as a tool for identifying novel selective ligands for FKBP51 generating the basis for the development of novel therapeutics.

Reference:

[1] Lerma Romero *et al.* Front. Mol. Biosci. (2022) 9:1023131. doi: 10.3389/fmolb.2022.1023131

Fragment-based drug design for the development of new antituberculosis drugs

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The rising number of people dying with tuberculosis, caused primarily by Mycobacterium tuberculosis (Mtb), and the appearance of extensively-drug resistant strains leads to an urgent need for new antituberculosis drugs with alternative modes of action [1]. As part of the thioredoxin (Trx) system, thioredoxin reductase of MTb (MTb-TrxR) is part of the oxidative defense and is essential for bacterial survival. Therefore, TrxR is a promising new target for the development of new therapeutics, as its druggability has already been proven [2].

For the identification of new fragment-based starting points and the investigation of new interaction sites for potential drugs, a crystallographic fragment screening was performed using 96 compounds of the F2X-Entry Screen and the largely automated software pipeline at HZB [3].

With a hit rate of 42%, four interesting binding sites were found at key interaction sites, showing a high potential for possible inhibition. Two fragments were selected and optimized using two different computational methods, after only one round of optimization a compound with µM inhibitory activity was found, and the binding position was confirmed.

References:

[1] Geneva: World Health Organization, *Global tuberculosis report 2021*, **2021**.

[2] a) O. Koch, L. Bering, EP 17 179 568.5 filed 04th July **2017** & PCT/EP2018/066768 filed 22nd June **2018**; b) K. Lin et al., *PLoS pathogens*, *12*, e1005675, **2016**; c) O. Koch et al., *J. Med. Chem.*, *56*, 4849, **2013.**

[3] a) G. M. A. Lima et al., *Acta Crystallogr. D*, *77*, 799, **2021**; b) U. Mueller et al., *Eur. Phys. J. Plus*, *130,* **2015**; c) J. Wollenhaupt et al., *JoVE,* **2021**; d) J. Wollenhaupt et al., *Structure (London, England: 1993)*, *28*, 694-706.e5, **2020.**

Quantifying the magnetic anisotropy of magnetic nanoparticles in biological vehicles

L. Marcano[1], I. Orue[2], D. Gandia[3], L. Gandarias[4], M. Weigand[5], Radu M. Abrudan[5], A. García Prieto[6], A. García-Arribas[3,7], A. Muela[4], M. L. Fdez-Gubieda[3,7], S. Valencia[5]

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Over the last years, the interest in nanomagnets has risen aiming to overcome the fundamental need to develop novel nanotechnology-based pathways to achieve relevant performance in medicine. On the top of their reduced size, that allows promising interaction with biological systems, the magnetic nature of the nanomagnets grants their manipulation by external magnetic fields. All of it makes magnetic nanostructures excellent candidates to be used as theranostic agents, to locally heat and destroy cancer cells in hyperthermia cancer treatment or for targeted magnetic cell delivery in regenerative medicine [1]. All these applications rely on the underlying physical properties of the nanomagnets within the target biological entity. In particular, the role of the magnetic anisotropy arises an overriding issue [2]. Despite its importance, the quantification of the magnetic anisotropy of individual magnetic nanostructures is a challenging task. Commonly used macroscopic magnetic characterization techniques impede obtainning reliable information about magnetic anisotropy of individual nanostructures. On the other hand, magnetic sensitive microscopic methods, they are either limited in spatial resolution, in magnetic field strength or more relevant, they do not allow to measure magnetic signals of nanomagnets embedded in biological systems. Here we present a hybrid experimental/theoretical method capable of working out the magnetic anisotropy constant and the magnetic easy axis direction of individual nanomagnets embedded in biological entities [3]. The method combines experimental data acquisition by means of scanning transmission x-ray microscopy (STXM) using an axi-asymmetric magnetic field with theoretical simulations based on the Stoner-Wohlfarth model. The imposed axi-asymmetric experimental magnetic field condition reduce the correlation between the parameters involved and facilitates the theoretical analysis while improves the accuracy of the results. The validity of the method has been tested over a model system consisting on single-domain intracellular magnetite nanoparticles biosynthesized by magnetotactic bacterium *Magnetovibrio blakemorei* MV-1.

References:

[1] Q. A. Pankhurst, et al., J. Phys. D: Appl. Phys., 36 (2003) R167–R181.
[2] D. Lisjak and A. Mertelj, Prog. Mater. Sci., 95 (2018) 286–328.
[3] L. Marcano, I. Orue, D. Gandia, et al., ACS Nano. 16 (2022) 7398-7408

In vivo detection of zinc-storing compounds in Drosophila utilizing X-ray absorption spectroscopy

Erika Garay[1†], Nils Schuth[1†], A. Barbanente[2], C. Tejeda-Guzmán[1], D. Vitone[2], B. Osorio[1], A. H. Clark[3], M. Nachtegaal[3], M. Haumann[4], H. Dau[4], A. Vela[1], Fabio Arnesano[2*], Liliana Quintanar[1*], Fanis Missirlis[1*]

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Zinc deficiency is commonly attributed to inadequate absorption of this metal. Instead, here we show that body zinc storage in Drosophila melanogaster depends on tryptophan (Trp) consumption. Our experiments showed (i) a correlation between the concentration of Trp metabolites in the diet and zinc concentration in Drosophila *in vivo* and (ii) that these metabolites can bind Zn *in vitro*. To our excitement, the XAS experiments conducted at the KMC-3 beamline at BESSY II provided the missing link by showing the presence of these *in vitro* zinc-storing compounds in the fly. Hence, dietary Trp regulates zinc status of the whole insect – a finding consistent with the widespread requirement of zinc as a protein cofactor. Our work presents a rare example (no equivalent precedent in the literature) where the endogenous ligands of a metal within an unperturbed biological specimen have been understood and described *in situ*.

Reference:

PNAS 119, 16 (2022)

PUBLIC LECTURE *17:00 - 18:00*

Thoughts About the Right Here, Right Now Global Climate Summit

Seth R. Marder

Renewable and Sustainable Energy Institute, Department of Chemical and Biological Engineering, Department of Chemistry, and Materials Science Program, University of Colorado Boulder, 027 UCB, Boulder, CO 80309, USA

UN Human Rights works to protect the rights and freedoms set forth by the Universal Declaration of Human Rights. The University of Colorado Boulder in collaboration with UN Human Rights and *Right Here, Right Now*, organized a global climate summit addressing the interconnectedness of human rights and climate change https://www.colorado.edu/globalclimatesummit/

While I'm neither an expert on climate change nor human rights I've had the privilege to be one of the co-Chairs of the Program Committee working with a talent steering committee, assisted by many other to create the agenda for this three-day summit:

Day 1: Impacts- The impacts of climate change on human rights

Day 2: Obligations- Understanding our human right responsibilities related to climate change

Day 3: Solutions- Develop policies and action items that are ground in human rights

Each day will have feature a keynote speaker:

- Sheila Watt Cloutier- A global advocate for Indigenous rights and health, will share her insight and experience as an Indigenous leader and the impact of climate change on human rights.
- President Mary Robinson- A respected advocate for climate justice and the former president of Ireland and UN High Commissioner on Human Rights, Mary will join the summit and discuss how to understand climate change as a matter of human rights.
- Kumi Naidoo- A life-long human rights advocate, Ninth Secretary-General of Amnesty International and Executive Director of Greenpeace. As a leader in climate solutions, education and advocacy, Naidoo will share his expertise on the summit's final day.

These keynotes are accompanied by 5 panels with world leading experts to discuss these issues in more depth.

When I give this presentation, the Summit will have just ended and I hope to share some impressions about what was learned, what lies ahead, and how you can become involved as part of the solution.

POSTER SLAM *15:00 - 16:00*

The virtual poster session will be accompanied by a thrilling poster slam. The poster slam offers a unique opportunity to present latest findings in a concise and entertaining way. A fast-paced poster slam allows each presenter one slide and 150 seconds to advertise their poster and tell the audience why the work is outstanding, important, and/or novel.

In the order of appearance:

1 PM2_VEKMAG / Matter & Material

Direct observation of the exchange anisotropy in the helimagnetic insulator Cu_2OSeO_3

Priya Ranjan Baral (EPFL, Switzerland)

The role of anisotropic exchange interaction (AEI) has been recently found to be crucial for the low-temperature phase diagram of chiral cubic magnet Cu_2OSeO_3. Transmission resonant x-ray scattering (t-REXS) in vector magnetic fields was utilized to directly quantify the temperature dependence of AEI in Cu_2OSeO_3. The AEI sharply increases below 35 K resulting in the conical spiral pitch variation of 10%.

2 PTB Laboratory at BESSY II / Other

Challenges in the traceable concentration measurement of nanoparticles by small angle X-ray scattering (SAXS)

Robin Schürmann (Physikalisch-Technische Bundesanstalt, Germany)

SAXS is a powerful tool for the traceable determination of nanoparticle (NP) concentrations by measurements of the scattering intensity in terms of SI-units. Here a novel approach is presented using SAXS with complementary techniques to determine the size distribution, density and number concentration of silica NPs with unknown electron density and compared with results from different methods.

3 UE56-1_SGM / Matter & Material

Soft-XAS Observation during CVD-Growth of Oxide Films: New Setup at UE56/1-SGM for Studies at Moderate Pressure

Stefan Cramm (Forschungszentrum Jülich, Germany)

The structure of CVD grown films depends on precursor gas pressure, growth temperature and, as recently observed, also on a magnetic field applied during growth. Detailed understanding of e.g. 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 TiO2 films from TTIP precursor are shown.

POSTER SLAM

4 BAMline / Energy Storage

In operando Computed X ray Tomography of abuse mechanisms in a commercial Li-Ion battery

Shahabeddin Dayani (Bundesanstalt für Materialforschung und -prüfung, Germany)

Thanks to their high brilliance, Synchrotron beams 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 poster we illustrate how one can utilize this ability to investigate abuse mechanisms on an actual commercially available lithium ion battery as well as a homemade.

5 KMC-3 / Energy Conversion

Investigation of oxidation state changes of Cobalt-based electrocatalyst by time-resolved operando X-ray absorption spectroscopy

Shima Farhoosh (Freie Universität Berlin, Germany)

Catalytic material undergoes oxidation state and structural changes during water oxidation. In this study, operando time-resolved XAS was employed to follow oxidation state changes in CoCat. X-ray absorption spectra were collected simultaneously with current response to various potential jumps. Time-resolved detection of X-ray signal revealed the kinetics of Co redox transitions.

6 PTB Laboratory at BESSY II / Life Science & Health

Quantitative analysis of trace elements in pancreatic carcinoma and pancreas sections of mice by reference-free X-ray Fluorescence analysis

Katja Frenzel (Physikalisch-Technische Bundesanstalt, Germany)

Reference-free X-ray fluorescence (XRF) analysis is a non-destructive method with a high sensitivity for a wide range of elements. The objective is to determine how the elemental mass distribution in benign pancreatic tissue differs compared to malignant pancreatic tissue. Quantifiable differences in mass deposition distribution in differently treated carcinoma sections are also investigated.

7 Matter & Material

Synthesis and Characterization of Nanocomposites for Environmental Remediation of Waste Water Contaminated with Pharmaceutically Active Ingredients

Joel Mwangi Gichumbi (Chuka University, Kenya)

The scarcity of high-quality fresh water is common in developing countries. The release of pharmaceutically active ingredients causes negative effects to ecosystems. Our research group is fabricating composites using nanomaterials and plant wastes which are studied for their adsorptive capacity in the removal of pollutants from waste water.

POSTER SLAM

8 MX Beamline / Life Science & Health

The Search for FGE Enhancing Molecules: Crystallographic Fragment Screen

Julia L. Kowal (Universität Bielefeld, Germany)

The formylglycine-generating enzyme modifies the active sites of human sulfatases. Destabilizing mutations lead to a lack of sulfatase modification and the rare disease multiple sulfatase deficiency. In a crystallographic fragment screen at BESSY BL 14.2 using the F2X-Entry Screen and 36 additional compounds, we revealed 12 unique fragment hits in 4 interaction sites.

9 PM4 / Life Science & Health

Structural Investigation of Ag nanoparticles with silane-functionalized TiO_2 nanoparticles for dual antibacterial effect

Martina Marsotto (RomaTre University, Italy)

In this research, our attention is mainly focused on the determination of the chemical composition and molecular structure of TiO_2@3MPTS-Ag@3MPS by synchrotron radiation-induced X-ray photoemission spectroscopy (SR-XPS). In particular, in SR-XPS measurements we planned to focus on Si 2p, Ti 2p and O 1s core level signals because they are expected to be indicative for the covalent binding of the NPs.

10 Life Science & Health

Solar-driven electrocatalytic reduction of Chromium (VI) in wastewater over Carbon-coated zero-valent Copper

Daisy Nyawira (Technical University of Kenya)

Waste generated from leather industries needs to be managed in an environmentally acceptable manner that mitigates chromium pollution. This study aims at synthesizing pristine graphene, nitrogen-doped graphene and boron-doped graphene coated zero-valent Cu nanoparticles to be used as electrocatalysts in the reduction of Cr(VI) to Cr(III). Cu nanoparticles will be synthesized via solvothermal and microwave.

11 PTB Laboratory at BESSY II / Energy Storage

Operando NEXAFS on Lithium Sulfur Batteries

Konstantin Skudler (Physikalisch-Technische Bundesanstalt, Germany)

Lithium Sulfur Batteries are with their high specific capacities and energy densities are promising alternatives to conventional lithium-ion batteries, yet there are some degradation mechanisms limiting their cycle stability. Within the project of the DFG Priority Programme Polymer-Based Batteries the goal is to monitor their degradation effects by Operando S-NEXAFS and increase their lifetime.

POSTER SLAM

12 ISISS / Energy Conversion

Ni-Fe/CeO_2-ZrO_2 bimetallic cermets as SOFC electrodes: In-situ ambient pressure-XPS and -NEXAFS studies in H_2 and CH_4 atmospheres

Lucia Maria Toscani (UNSAM-CONICET, Argentina)

Solid oxide fuel cells (SOFC) stand as a promising technology for efficient and clean energy production. Ni-Fe/CeO_2-ZrO_2 cermet exhibits Ni-Fe nanoparticles that promote H_2 and CH_4 oxidation reactions. Our in-situ NAP-XPS and NEXAFS study reveals surface changes when H_2 and CH_4 are used as fuels. We find a high catalytic activity for methane oxidation reaction and carbon formation resistance.

13 EMIL_CPMU17 / Energy Conversion

In situ P K-edge XANES Investigation of Interactions at the Pt/H_3PO_X Interface

Enggar Pramanto Wibowo (Helmholtz-Zentrum Berlin, Germany)

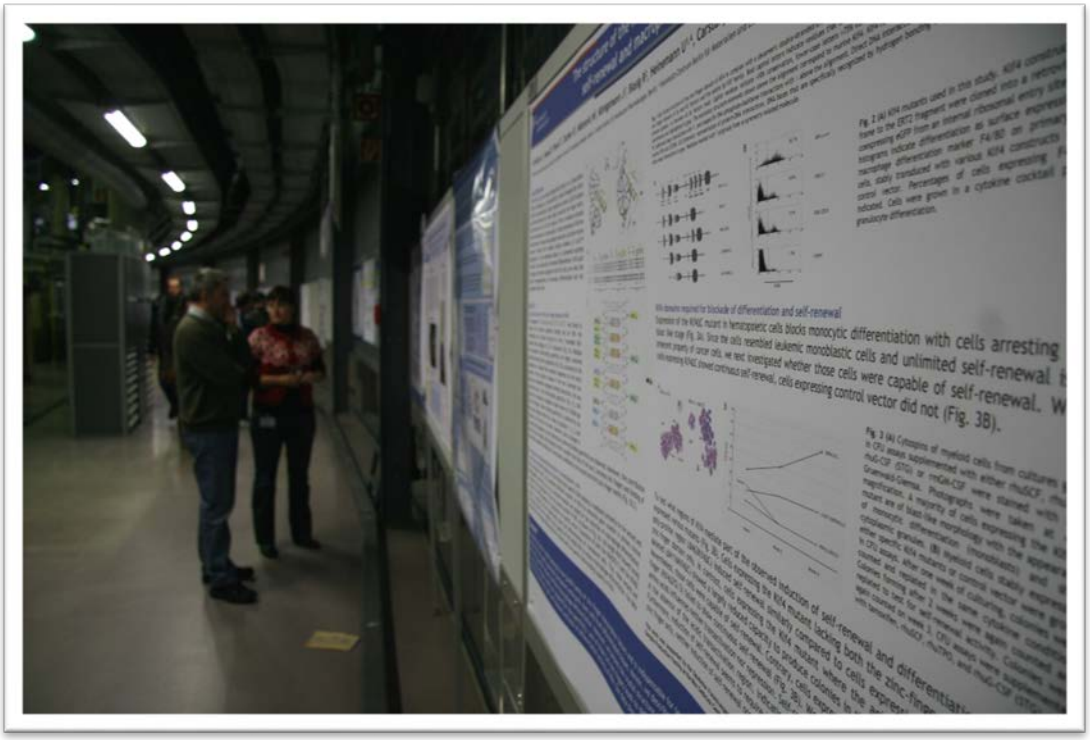
Recent studies suggest a possible reduction of H_3PO_4 to H_3PO_3 during the operation of HT-PEMFCs, which might poison the Pt catalyst. However, Pt also catalyzes the chemical oxidation of aq. H_3PO_3 to H_3PO_4, indicating the complexity of the Pt/H_3PO_X interaction. In this work, we gain insight on the Pt/H_3PO_X interface through in situ P K-edge XANES at experimental conditions relevant to HT-PEMFCs operation.

14 PTB Laboratory at BESSY II / Matter & Material

Moderate-Resolution XES using a full-cylinder von Hamos spectrometer

Kai Schüler (Physikalisch-Technische Bundesanstalt, Germany)

The alignment of the PTB's von Hamos spectrometer is critical to optimize the response function and the detection efficiency. For that reason, parametric optimization routines for enhanced alignment reliability and reproducibility were developed, which also consider the position of the optic and the sample position and base on geometrical reflection computations.



SCIENTIFIC TOPICS

Energy Conversion

Energy Storage

Information Technology

Life Science & Health

Matter & Material

Other

PTB Laboratory at BESSY II

XAS for structural characterization of atomically dispersed materials

Simon Dietzmann (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

Atomically dispersed metal-nitrogen doped carbons (M-N-C) are promising catalysts for small molecule activation. These materials are characterized by XAS to determine the coordination sphere around the metal.

In situ P K-edge XANES Investigation of Interactions at the Pt/H_3PO_X Interface

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Ni-Fe/CeO_2-ZrO_2 bimetallic cermets as SOFC electrodes: In-situ ambient pressure-XPS and -NEXAFS studies in H_2 and CH_4 atmospheres

Lucia Maria Toscani (UNSAM-CONICET, Argentina) ***ISISS***

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Surface and Interface Study of Hybrid Perovskite Top Cells in Tandem Devices for Revealing the Impact of Omitting the ALD deposited SnO_2 Buffer Layer

Elif Hüsam (Helmholtz-Zentrum Berlin, Germany) ***KMC-1***

Wide-bandgap metal halide perovskites (HaPs) are used as photoactive absorber layers in tandem solar cells. Interface formations between absorber and electron transport layers (ETL) crucially influence device properties, thus we comprehensively studied the buried interfaces formed in HaP half-cells with different stacks of ETL by HAXPES at the HiKE endstation.

Calculation of the lead-halide distance distribution of MAPbX3 from experimental Morse potential data

Götz Schuck (Helmholtz-Zentrum Berlin, Germany) ***KMC-2***

Morse potential parameters can be obtained from temperature-dependent EXAFS data on chlorine-substituted MAPbI3. The Morse potential parameters in turn allowed for a comparison of the experimental results shown here with other experimental methods as well as with DFT calculations as described in the literature. The EXAFS results can be used as a benchmark for theoretical calculations.

Investigation of oxidation state changes of Cobalt-based electrocatalyst by time-resolved operando X-ray absorption spectroscopy

Shima Farhoosh (Freie Universität Berlin, Germany) *KMC-3*

Catalytic material undergoes oxidation state and structural changes during water oxidation. In this study, operando time-resolved XAS was employed to follow oxidation state changes in CoCat. X-ray absorption spectra were collected simultaneously with current response to various potential jumps. Time-resolved detection of X-ray signal revealed the kinetics of Co redox transitions.

Rapid-scan operando-XAS at beamline KMC-3

Michael Haumann (Freie Universität Berlin, Germany) *KMC-3*

KMC-3 is a versatile bending magnet beamline at BESSY. Recent developments include rapid-scan XAS in seconds with a 13-element energy resolving detector, XAS at the P and S K-edges down to 2 keV, and operando-XAS combined with electrochemistry. The recent developments are outlined and future extensions of the XAS experiment are discussed.

Insights into the structural changes of amorphous and crystalline iridium oxides under Oxygen Evolution Reaction (OER) conditions by operando Ir L3-edge XANES and EXAFS

Marianne van der Merwe (Helmholtz-Zentrum Berlin, Germany) *KMC-3*

The anti-correlation between OER activity and stability of iridium oxide electrocatalysts is associated with their degree of crystallinity and hydration. In this operando XAS study at Ir L3-edge, we reveal the potential-induced spectroscopic changes of several commercial amorphous and crystalline iridium oxides under OER conditions, and link the nature of the redox processes to the oxidation state changes

Oxide evolution in copper foams for electrochemical CO_2 reduction tracked by operando X-ray absorption and operando Raman spectroscopy

Fan Yang (Freie Universität Berlin, Germany) *KMC-3*

Surface-sensitive operando Raman spectroscopy and bulk-sensitive operando X-ray absorption spectroscopy (XAS) are combined to track oxide evolution of Cu foams under electrochemical conditions. Based on this study, we hope to explore the role of copper oxides in the reduction of carbon dioxide.

Direct probing of the long-lived photoexcited state in a prototypical Ni catalyst

Rachel Wallick (University of Illinois at Urbana Champaign, US) *UE52_SGM*

Herein we present ultrafast L-edge X-ray absorption spectroscopy of a prototypical Ni photocatalyst. A long-lived excited state with a 4 ns lifetime has been identified via optical studies, but the identity of this state is unknown. We show that it is a triplet tetrahedral metal-centered state. This will lend insight into Ni photocatalytic cycles, which are debated in the literature.

Solar-to-Ethanol production: The sustainable synthesis of green ethanol for cooking fuel

Nancy Khayongo Ochiba (Technical University of Kenya)

Anthropogenic CO_2 greatly contributes to global warming, consequently climate change. Electrocatalytic reduction of CO_2 in the presence of green hydrogen for synthesis of green ethanol is one of most propitious technologies that'll reverse adverse climatic changes. This approach may reduce over-reliance on fossil fuels. The study aims at the synthesis of green ethanol for cooking *via* the electrocatalytic reduction of CO_2 in the presence of green hydrogen.

Thermolysis of SURMOF ZIF-67 thin film: a combined in situ IRRAS, XPS, and NEXAFS study

Jimin Song (Karlsruhe Institute for Technology, Germany)

Through a pyrolysis treatment, ZIF-67 derived materials are very promising catalysts in the energy conversion related reactions. However, the evolution of ZIF-67 in the pyrolysis process remains still unclear. Annealing in UHV chambers, in situ IRRAS, XPS and NEXAFS were applied to uncover the temperature dependent evolution of ZIF-67 from 300K to 900K.

In operando Computed X ray Tomography of abuse mechanisms in a commercial Li-Ion battery

Shahabeddin Dayani (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

Thanks to their high brilliance, Synchrotron beams 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 poster we illustrate how one can utilize this ability to investigate abuse mechanisms on an actual commercially available lithium ion battery as well as a homemade.

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

Zora Chalkley (Helmholtz-Zentrum Berlin, Germany) ***KMC-1***

In anode-free lithium 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. Modifications to the battery design, which are required to conduct such an experiment, are presented using two solid polymer electrolyte AFLMBs.

X-ray zoom lens at BAMline

Arndt Last (Karlsruhe Institute for Technology, Germany) ***BAMline***

A motorized X-ray zoom lens from KIT/IMT based on a polymer compound refractive X-ray lens (CRL) fabricated via deep X-ray lithography at the synchrotron source KARA has been installed and tested at BAMline. First experiences will be reported.

Functionalized Fullerene for Inhibition of SARS-CoV-2 Variants

Ievgen Donskyi (Freie Universität Berlin, Germany) ***HE-SGM***

Here, we combined hydrophobic fullerene with the polyglycerol sulfate to inhibit infection of SARS-CoV-2 variants in vitro. Samples were characterized with different methods, including XPS and NEXAFS. Effective inhibitory concentrations in the nanomolar range highlight the significance of bare fullerene's hydrophobic moiety and electrostatic interactions of polysulfates with surface proteins of SARS-CoV-2.

Update on Microscopy and Imaging at IRIS beamline

Ljiljana Puskar (Helmholtz-Zentrum Berlin, Germany) ***IRIS***

The IRIS microscopy station provides chemical information spanning spatial resolution from nm to µm. Presented here is the latest status and applications of the IRIS diffraction limited IR microscope (5-10 µm lateral resolution in MIR) equipped with both single point and imaging (64x64) FPA detectors and polarization modulation options, operating in both MIR and FIR regions.

Hundreds of starting points to develop protein-protein interaction modulators

Tatjana Bartel (Helmholtz-Zentrum Berlin, Germany) ***MX Beamline***

Crystallographic fragment screening facilitates the identification of weak but efficient small molecules (fragments) while elucidating their binding mode and position. This enables structure-guided optimization of bound fragments into potent modulators. Here, the ~1000-fragment large F2X-Universal Library was screened against a spliceosomal protein-protein complex and resulted in hundreds of hits.

NECESSITY - New chemical entities for modulating SARS-CoV-2 activity

Leila Benz (Helmholtz-Zentrum Berlin, Germany) ***MX Beamline***

To combat the still ongoing SARS-CoV-2 pandemic more potent anti-viral drugs are needed. The collaborative NECESSITY project aims at screening the main protease of the virus in an x-ray crystallographic compound screening campaign against a unique library of over 8000 small molecule compounds to find potential inhibitors and to further test initial hits with biochemical and biophysical methods.

Lipase B from Candida antarctica: Conformation and Mechanism

Jaroslaw Blaszczyk (CMMS, Polish Academy of Sciences, Poland) ***MX Beamline***

Candida antarctica Lipase B (CAL-B) is one of the most extensively used biocatalysts in stereoselective synthesis. CAL-B also shows a promiscuous activity. Earliest reports about CAL-B crystal structure are dated between 1994-95. The structures solved a quarter-a-century gap after that, give a hint of the enzyme mechanism in three dimensions.

Crystallization of bacterial histidine kinase in complex with ATP analogues

Anna Cociurovscaia (Lodz University of Technology, Poland) ***MX Beamline***

The CusS histidine kinase belongs to the bacterial two-component regulatory system CusSR, responsible for the synthesis of copper efflux pump. The first crystal structure of the CusS kinase core was solved at 1.4 Å, allowing the identification of catalytic motifs engaged in the phosphorylation mechanism. Currently, trials aiming to obtain the transient ATP-bound kinase conformation constitute our main goal.

The Search for FGE Enhancing Molecules: Crystallographic Fragment Screen

Julia L. Kowal (Universität Bielefeld, Germany) ***MX Beamline***

The formylglycine-generating enzyme modifies the active sites of human sulfatases. Destabilizing mutations lead to a lack of sulfatase modification and the rare disease multiple sulfatase deficiency. In a crystallographic fragment screen at BESSY BL 14.2 using the F2X-Entry Screen and 36 additional compounds, we revealed 12 unique fragment hits in 4 interaction sites.

How does Watson-Watson differ from Watson-Crick?

Petr Kolenko (Czech Technical University Prague, Czech Republic) ***MX Beamline***

Watson-Crick base pairs are building blocks of double-stranded DNA molecules, the genetic material of a cell. The synthesized molecules in the cell undergo proofreading to prevent mutations. We aim to understand structural differences of non-canonical Watson-Crick base pairs to better understand the proofreading process. As a target, DNA 18-mers accommodating double mismatches were chosen.

Searching for inhibitors targeting Rab-GAP interactions

Dominika Krzeszewska (Lodz University of Technology, Poland) ***MX Beamline***

Rab proteins belong to the superfamily of small GTPases responsible for maintaining the vesicular transport. GAP proteins downregulate Rabs by stimulating their intrinsic GTPase activity. People with metabolic diseases often have the reduced activity of Rabs, hence molecules targeting Rab-GAP interactions are sought. For this purpose, an analysis of protein crystal structures is crucial.

Crystal structure of bifunctional transacetylase from Arabidopsis thaliana (AtNAOGAT) – an enzyme of arginine cyclic biosynthesis pathway

Maciej Nielipinski (Lodz University of Technology, Poland) ***MX Beamline***

One of Arabidopsis' thaliana still not characterized proteins is AtNAOGAT, a bifunctional transacetylase, active in ornithine synthesis pathway and arginine synthesis cyclic pathway. While produced as a whole, it undergoes autoproteolysis forming subunits α and β. Preliminary analysis of orthologous structures indicate biological assembly of dimer of heterodimers αβ.

Structures of a DYW domain indicate a unique plant RNA editing regulation principle

Gert Weber (Helmholtz-Zentrum Berlin, Germany) ***MX Beamline***

We have obtained first structures of a plant RNA editosomal DYW deaminase domain which shed light on a unique regulation mechanism for metalloproteins. Activity of the deaminase functionis geared by structural changes around a catalytic Zn-atom with respect to its coordination. These observations are in line with our biochemical data supporting an activation mechanism for DYW domains.

Fragment screening workflow for MX users

Jan Wollenhaupt (Helmholtz-Zentrum-Berlin, Germany) ***MX Beamline***

At the macromolecular crystallography beamlines at HZB, a workflow including dedicated tools, highly diverse compound libraries and software solutions was established and optimized to provide for efficient fragment screening. Bound fragments are identified in a largely automated fashion and can be optimized readily with our growing by catalog approach for tool compound development and drug design.

Structural Studies on New Factors Involved in Histone mRNA Decay – UPF2 and 3'hExo

Guangpu Xue (Freie Universität Berlin, Germany) ***MX Beamline***

The RNA helicase UPF1 plays a central role in nonsense-mediated mRNA decay (NMD) as well as other degradation pathways in eukaryotes. UPF2 is the activator of UPF1. In our current study, we have identified UPF2 as a player in histone mRNA decay. In addition to its association with UPF1, we find that UPF2 also binds 3'hExo, a 3'-5' exonuclease which is a core factor of the initial histone mRNA decay complex.

Structural Investigation of Ag nanoparticles with silane-functionalized TiO_2 nanoparticles for dual antibacterial effect

Martina Marsotto (RomaTre University, Italy) ***PM4***

In this research, our attention is mainly focused on the determination of the chemical composition and molecular structure of TiO_2@3MPTS-Ag@3MPS by synchrotron radiation-induced X-ray photoemission spectroscopy (SR-XPS). In particular, in SR-XPS measurements we planned to focus on Si 2p, Ti 2p and O 1s core level signals because they are expected to be indicative for the covalent binding of the NPs.

Solar-driven electrocatalytic reduction of Chromium (VI) in wastewater over Carbon-coated zero-valent Copper

Daisy Nyawira (Technical University of Kenya)

Waste generated from leather industries needs to be managed in an environmentally acceptable manner that mitigates chromium pollution. This study aims at synthesizing pristine graphene, nitrogen-doped graphene and boron-doped graphene coated zero-valent Cu nanoparticles to be used as electrocatalysts in the reduction of Cr(VI) to Cr(III). Cu nanoparticles will be synthesized via solvothermal and microwave.

Field-Induced modification on the electronic structure in BTBT-based organic thin films

Rainer Fink (FAU Erlangen-Nürnberg, Germany) ***HE-SGM***

We present an in-operando NEXAFS study on BTBT-based self assembled monolayer films. We observe field-induced modifications in the NXAFGS spectra. Variations in the on- and off-states are interpreted in the context of polaron formation due to charge accumulation induced by the applied electric field.

Biopolymers polylactic acid and polyhydroxybutyrate covered with thin amorphous hydrogenated carbon films - Substrate chemistry impact on interlayer formation

Torben Schlebrowski (Universität Koblenz, DE) ***HE-SGM***

To adapt a polymeric material for different applications, it can be coated with amorphous hydrogenated carbon layers (a-C:H). During layer deposition, a mixed phase (=interlayer) is formed. The influence of the base material on the interlayer formation during coating is examined using the polylactide (PLA) and polyhydroxybutyrate (PHB), which have a quite similar chemical composition.

Multiscale investigation of cellulose using infrared spectroscopy methods

Alexander Veber (Humboldt Universität Berlin, Germany) ***IRIS***

Cellulose was studied using IR spectroscopy techniques at different spatial scales: conventional FTIR, diffraction limited and tip-enhanced IR micro- and nanospectroscopy. The multiscale characterization of cellulose demonstrates capabilities and complementarity of different infrared spectroscopy methods for characterization of hierarchical and complex composite materials at different spatial scales.

Instrumentation for monitoring of stimuli-induced phase transitions in photoswitchable nanoporous solids

Volodymyr Bon (Technische Universität Dresden, Germany) ***KMC-2***

Herein we present the dedicated instrumentation for monitoring guest- and light-induced phase transitions in switchable nanoporous solids by in situ PXRD, developed at KMC-2 beamline. The first results on the dynamic guest-responsive framework DUT-137 with embedded photoactive azo-groups are discussed.

Laser-induced magnetic phase transition of FeRh studied by UXRD and MOKE

Maximilian Mattern (Universität Potsdam, Germany) ***KMC-3***

We present ultrafast x-ray diffraction (UXRD) and magneto-optical Kerr effect (MOKE) measurements that probe the laser-induced metamagnetic phase transition in homogeneously and inhomogeneously excited FeRh thin film samples. Their comparison provide insight into the intrinsic evolution of the order parameters of the laser-induced FM phase.

KMC-3 XPP: Time-resolved Hard X-ray Diffraction at BESSY II

Matthias Rössle (Helmholtz-Zentrum Berlin, Germany) *KMC-3*

The XPP endstation at the KMC-3 beamline is optimised for the investigation of the structural response of matter with ps time-resolution after an optical laser or electrical pulse excitation of thin films or layered heterostructures. We present the experimental setup and demonstrate the ultrafast structural response showing different excitation and detection schemes available at KMC-3 XPP.

EXAFS spectroscopy and diffusion phenomena in CrMnFeCoNi single crystals

Alevtina Smekhova (Helmholtz-Zentrum Berlin, Germany) *KMC-3*

The multi-edge EXAFS spectroscopy combined with reverse Monte Carlo (RMC) simulations was used to probe the details of local coordination and component-dependent structure relaxations in single crystalline CrMnFeCoNi high-entropy alloy. Both states – homogenized at high-temperature and further annealed at 720°C for 14 days – reveal correlations with fundamental characteristics of element diffusion.

Polymorphism in molecular cocrystals controlled by variable temperature ball milling

Kevin Linberg (Bundesanstalt für Materialforschung und -prüfung, Germany) *mySpot Beamline*

Mechanochemistry offers a unique opportunity to modify or synthesize new crystal forms. Although the method is very promising, little is known about the mechanochemical means to control the synthesis of a solid form. Using an polymorphic organic cocrystal system, we show here that mechanochemistry can be used to obtain a polymorph transformation under the apparently conventional (thermal) transition point.

Direct observation of the exchange anisotropy in the helimagnetic insulator Cu_2OSeO_3

Priya Ranjan Baral (EPFL, Switzerland) *PM2-VEKMAG*

The role of anisotropic exchange interaction (AEI) has been recently found to be crucial for the low-temperature phase diagram of chiral cubic magnet Cu_2OSeO_3. Transmission resonant x-ray scattering (t-REXS) in vector magnetic fields was utilized to directly quantify the temperature dependence of AEI in Cu_2OSeO_3. The AEI sharply increases below 35 K resulting in the conical spiral pitch variation of 10%.

Comparison of spin-crossover properties between thin film and bulk sample of a binuclear Fe(II) complex

Marcel Walter (Freie Universität Berlin, Germany) *PM2-VEKMAG*

We deposit large spin-crossover molecules (SCMs) on solid surfaces using a pulsed-valve vapor deposition method. This has the advantage that no thermal energy is applied to the SCMs. X-ray absorption spectroscopy at the VEKMAG beamline is used to examine cooperative behavior in the spin switching of a dinuclear SCM. The results show a similar switching behavior as in the bulk material.

Surface-assisted synthesis of nanographenes: Cyclodehydrogenation of 1,1'-bitetracene to peri-tetracene

Maren Klein (Universität Tübingen, Germany) ***PM4***

Periacenes can be considered as zigzag shaped nanographene units with attractive electronic properties for future electronic devices. They can be formed via on-surface synthesis, which could be a promising route for the synthesis of related molecules and thus the band-gap tuning of nanographenes. Studies indicate that the newly synthesized 1,1'-bitetracene can undergo such a cyclodehydrogenation on Cu(111).

Long-term degradation mechanisms in Blatter radical derivative thin films

Ewa Nowik-Boltyk (Universität Tübingen, Germany) ***PM4***

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.

Correlative studies of MoVTeNb oxides by in-situ TXM and TEM

Kassiogé Dembélé (Fritz-Haber-Institut, Germany) ***U41-TXM***

We studied chemical changes induced by temperature and gas composition on MoVTeNb oxides. Using the in-situ TEM, we did not observe significantly change in the particles morphology during the introduction of the propane in the synthetic air and the consecutive heating to 420 °C. However, the local XAS indicated changes in the oxidation state of vanadium due to the applied gas and temperature.

Soft-XAS Observation during CVD-Growth of Oxide Films: New Setup at UE56/1-SGM for Studies at Moderate Pressure

Stefan Cramm (Forschungszentrum Jülich, Germany) ***UE56-1_SGM***

The structure of CVD grown films depends on precursor gas pressure, growth temperature and, as recently observed, also on a magnetic field applied during growth. Detailed understanding of e.g. 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 TiO2 films from TTIP precursor are shown.

Synthesis and Characterization of Nanocomposites for Environmental Remediation of Waste Water Contaminated with Pharmaceutically Active Ingredients

Joel Mwangi Gichumbi (Chuka University, Kenya)

The scarcity of high-quality fresh water is common in developing countries. The release of pharmaceutically active ingredients causes negative effects to ecosystems. Our research group is fabricating composites using nanomaterials and plant wastes which are studied for their adsorptive capacity in the removal of pollutants from waste water.

Upgraded imaging capabilities at the BAMline

Henning Markötter (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

A recent upgrade of key equipment of the BAMline widens 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 easily be set up. In fact, the upgraded double-multilayer monochromator brings full flexibility by yielding different energy spectra to optimize flux and energy resolution as desired.

Surface modification of polyhydroxybutyrate (PHB) by angle-dependent O2 plasma treatment

Lukas Beucher (Universität Koblenz, Germany) ***HE-SGM***

The O2-plasma treatment of biodegradable PHB, previously thought to be a cleaning process, alters surface properties. Similarly, the angle of incidence of the plasma-enhanced chemical vapour deposition to the sample surface affects the parameters such as contact angle, water vapor permeability, and chemical composition.

Occurence of persistent environmental pollutants in freshwater

Luisa Jordao (Instituto Nacional de Saude Dr Ricardo Jorge, Portugal) ***IRIS***

Freshwater pollution is a huge concern. Occurence of 2 groups of persistent pollutants with similar chemical properties (polycyclic aromatic hydrocarbons and microplastics) in Alqueva's surface water were evaluated during 2021. Samples were collected, once per season, at 3 spots related to touristic activities. Biofilm presence on plastic and natural materials was monitored and compared.

RIXS at PEAXIS - Determining the Electronic Structure of Solid-State Energy and Quantum Materials

Christian Schulz (Helmholtz-Zentrum Berlin, Germany) ***U41-PEAXIS***

Materials for energy and quantum applications benefit from their complex electronic structure. PEAXIS provides RIXS spectroscopy which is ideally suited to study electronic structure and dynamics of these materials. PEAXIS offers various features which allow to study electronic properties in a wide temperature range, with applied voltages and under continuous motion for X-ray sensitive samples.

Developments in sample preparation, handling, and storage in cryoEM

Joyce Frank (MiTeGen, Ithaca, US)

Interest in cryoelectron microscopy (cryoEM) is growing rapidly as technical advances in electron detectors and optics dramatically improve imaging capabilities and sample throughput. Systems for the advanced storage, transport, and tracking of cryo-EM samples are being developed. We report on our current and planned developments in this area.

SECoP@HMC - Metadata in the Sample Environment Communication Protocol

Klaus Kiefer (Helmholtz-Zentrum Berlin, Germany)

The International Society for Sample Environment (ISSE) developed the Sample Environment Communication Protocol (SECoP) to standardize the communication between instrument control software and SE equipment. SECoP offers, on the one hand, a generalized way to control SE equipment. On the other hand, SECoP holds the possibility to transport SE metadata in a well-defined way.

SyncLab combines laboratory spectrometers for 3D elemental imaging and soft NEXAFS with synchrotron experiments

Ioanna Mantouvalou (Helmholtz-Zentrum Berlin, Germany)

We present first application examples of measurements which use both laboratory equipment and synchrotron instrumentation. The added benefits are highlighted and further opportunities discussed.

Why less is more

Antonia Rötger (Helmholtz-Zentrum Berlin, Germany)

What can we learn from research on science communication? Is there advice for better exchange among scientists as well?

PTB LABORATORY AT BESSY II

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

Jérôme Deumer (Physikalisch-Technische Bundesanstalt, Germany)

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 this ensemble to calculate the single-particle SAXS pattern.

Quantitative analysis of trace elements in pancreatic carcinoma and pancreas sections of mice by reference-free X-ray Fluorescence analysis

Katja Frenzel (Physikalisch-Technische Bundesanstalt, Germany)

Reference-free X-ray fluorescence (XRF) analysis is a non-destructive method with a high sensitivity for a wide range of elements. The objective is to determine how the elemental mass distribution in benign pancreatic tissue differs compared to malignant pancreatic tissue. Quantifiable differences in mass deposition distribution in differently treated carcinoma sections are also investigated.

Tender X-ray micro focus beamline in the PTB Laboratory

Matthias Müller (Physikalisch-Technische Bundesanstalt, Germany)

PTB is currently installing a new beamline at the dipole 6.12 of BESSY II. The beamline will deliver radiation in the energy range from 1.5 keV - 8.0 keV with high spectral purity and stability for metrology and x-ray spectrometry. The diameter of the beam spot usable for the experiments can be varied from 5 µm to 40 µm. A combination of a PGM and a DCM will be employed to cover the tender X-ray range.

Moderate-Resolution XES using a full-cylinder von Hamos spectrometer

Kai Schüler (Physikalisch-Technische Bundesanstalt, Germany)

The alignment of the PTB's von Hamos spectrometer is critical to optimize the response function and the detection efficiency. For that reason, parametric optimization routines for enhanced alignment reliability and reproducibility were developed, which also consider the position of the optic and the sample position and base on geometrical reflection computations.

Challenges in the traceable concentration measurement of nanoparticles by small angle X-ray scattering (SAXS)

Robin Schürmann (Physikalisch-Technische Bundesanstalt, Germany)

SAXS is a powerful tool for the traceable determination of nanoparticle (NP) concentrations by measurements of the scattering intensity in terms of SI-units. Here a novel approach is presented using SAXS with complementary techniques to determine the size distribution, density and number concentration of silica NPs with unknown electron density and compared with results from different methods.

PTB LABORATORY AT BESSY II

Grazing emission X-ray fluorescence (GEXRF) for the characterization of advanced nanostructures

Dieter Skroblin (Physikalisch-Technische Bundesanstalt, Germany)

The grazing emission X-ray fluorescence technique offers a promising approach to determining the spatial distribution of various chemical elements in nanostructures. The angle-resolved fluorescence emission is collected with photon-counting hybrid pixel area detectors using scanning-free detection schemes. We demonstrate how this method can be used to characterize periodic TiO2 nanostructures.

Operando NEXAFS on Lithium Sulfur Batteries

Konstantin Skudler (Physikalisch-Technische Bundesanstalt, Germany)

Lithium Sulfur Batteries are with their high specific capacities and energy densities are promising alternatives to conventional lithium-ion batteries, yet there are some degradation mechanisms limiting their cycle stability. Within the project of the DFG Priority Programme Polymer-Based Batteries the goal is to monitor their degradation effects by Operando S-NEXAFS and increase their lifetime.

Quantitative element-sensitive analysis of individual nanoobjects

André Wählisch (Physikalisch-Technische Bundesanstalt, Germany)

X-ray fluorescence microscopy is an element-sensitive and non-destructive tool for the investigation of a wide range of nanotechnological materials. We show that a traceable quantification of individual nanoobjects can be realized when utilizing rather conventional but well-calibrated instrumentation. As a proof of concept, the total number of atoms forming a germanium nanoobject is quantified.

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

Nils Wauschkuhn (Physikalisch-Technische Bundesanstalt, Germany)

The complexity of today's nanostructures, especially for semiconductor-related applications, necessitates new metrology techniques. Here, the capability of scanning-free grazing emission X-ray fluorescence (GEXRF) will be demonstrated on two-dimensional nanostructures. TiO_2 gratings with variable etching depth, coated with HfO_2, are being characterized dimensionally and analytically.

Procedure for electing members of the HZB User Committee

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

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

The voting period for the HZB User Committee is

26. November 2022 [00:01 CET] - 09. December 2022 [23:59 CET]

Eligible users are defined as users of HZB facilities, who have been actively registered in the HZB access portal GATE as a proposer, co-proposer or user during the three years immediately preceding the election. All eligible users are informed in advance via email by the election committee. In order to be able to vote, the users must be registered in GATE.

The candidates for the legislative term 2023/24 are

Franziska Emmerling	Bundesanstalt für Materialforschung und -prüfung, Germany
Christian Gollwitzer	Physikalisch Technische Bundesanstalt, Germany
Heiko Peisert	Eberhard Karls Universität Tübingen, Germany
Michael Weyand	Universität Bayreuth, Germany

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

The members of the current election committee are

Wolfram Calvet	TU Darmstadt	Member of HZB User Committee
Olaf Schwarzkopf	HZB	Representative of HZB Director's Office
Beatrix-Kamelia Menzel	HZB	Representative of HZB User Coordination

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

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

Friends of Helmholtz-Zentrum Berlin e.V.

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

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

All natural or juristic persons may become member of the association. The regular annual membership fee amounts to 10 € for undergraduate and graduate students, 40 € for other natural persons and, as a rule, 150 € for juristic persons. In its work, the association depends also on donations which can also be addressed with a specific purpose, such as "Ernst-Eckhard-Koch-Prize" (Account-No: 414 44 40 at the Deutsche Bank AG, BLZ 100 700 00, IBAN: DE48 1007 0000 0414 4440 00, BIC: DEUTDEBBXXX). Fees and donations are enjoying tax privileges.

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

The Board of the Association

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

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

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

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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 September 2023 to February 2024.

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

http://hz-b.de/gate

DEADLINE
March 1st, 2023