HZB Helmholtz Zentrum Berlin
BESSY II

12th BESSY@HZB USER MEETING

December 10th, 2020

PUBLIC LECTURE

Rolf Hilgenfeld (DZIF)

INVITED TALKS

ENERGY CONVERSION

Ian Sharp (TUM)

ENERGY STORAGE

Sun Fu (QIBBT)

INFORMATION TECHNOLOGY

Yoav W. Windsor (FHI)

LIFE SCIENCE & HEALTH

Christian Feiler (HZB)

MATTER & MATERIAL

Rebecka Lindblad (Uni Uppsala)

POSTER SESSION POSTER SLAM VENDOR EXHIBITION

WELCOME

Dear Users and Friends,

Welcome to the 12th BESSY@HZB User Meeting 2020

We are all experiencing turbulent times and, as so many other events, our User Meeting is also affected by the ongoing pandemic. While meeting you in person is for us a highlight of the year, this year we have to change and to meet in the virtual space for the first time: no face-to-face conversations, no stimulatory coffee breaks and regrettably no “Berliner Buffet”. Nevertheless, we did not want to miss out on the opportunity of getting in touch with you, our users, and hope for a vivid exchange also in the new virtual format of the meeting.

The new coronavirus SARS-CoV-2 is keeping the world in suspense and as an international science hub, we are taking our responsibility in times of this pandemic very seriously. On the one hand, this implies constantly adjusting the user service to the status of the pandemic to protect users and staff from possible infections. Unfortunately, this meant that we were forced to impose restrictions and cancel or postpone beamtime campaigns. On the other hand, BESSY II is a precious tool for research about the virus, which might bring us closer to an effective vaccine or treatment. Therefore, we are offering priority fast track access for projects directly related to SARS-CoV-2 - this enabled selected measurements even during the most restricted times of the lockdown in spring. And we are glad to report that since the beginning of the pandemic, BESSY II was able to make very important contributions to SARS-CoV-2 research.

In February, Prof. Dr. Rolf Hilgenfeld, a globally renowned biochemist and structural virologist, and his team from the University of Lübeck decoded the 3D architecture of the viral main protease of SARS-CoV-2, based on measurements at BESSY II. The protein is involved in the reproduction of the virus, and analysing its architecture allows for the identification of specific points of attack for active substances and the systematic development of drugs which inhibit its reproduction. A major breakthrough that science can build on!

New collaborative research projects have been initiated to combat the virus. One project focussing on fragment-screening of the viral main protease has been started, encompassing teams from University of Lübeck, Julius-Maximilians-Universität of Würzburg and HZB. In a second project, a team from HZB and a Berlin biotech company have initiated a consortium of regional research groups to search for antiviral substances. The goal in both projects is to identify starting points for the development of potential drugs against SARS-CoV-2.

During the past year we also continued to work very successfully on topics other than Corona. We established new collaborations and strengthened our partnership with Universities through new joint research groups. Together with TU Berlin we will investigate how X-ray experiments on smaller laboratory instruments can be optimally complemented with experiments at synchrotron sources like BESSY II. The University of Kassel and HZB are setting up a joint laboratory for the use of artificial intelligence, where they will develop new methods and improve the analysis of data from experiments performed at BESSY II.

WELCOME

In cooperation with the Leibnitz-Institut für Kristallzüchtung we bundle our competencies in energy and quantum materials and plan to develop new types of X-ray optics for synchrotron radiation sources.

The User Meeting will again underline the broad variety of scientific fields addressed by the experiments realized by you at the HZB facilities. Once again, we have been able to attract outstanding speakers for five major focus areas: energy storage, energy conversion, life science & health, information technology and matter & materials. The Public Lecture on “Structure-based discovery of inhibitors of the SARS-CoV-2 main protease”, which Prof. Dr. Rolf Hilgenfeld kindly accepted to present, will certainly be a highlight of the program. Furthermore, we ask you to contribute your favourite method of virtual applause for the bestowal of the 'Prizes for Young Scientists'.

We will do our best to ensure that, despite its unusual format, this year’s User Meeting will further strengthen your interest in performing your research at BESSY II and initiate fruitful discussions, resulting in exciting experiments as well as new collaborations. Thank you all for joining us in these exceptional and turbulent times.

Enjoy the meeting!

Sincerely

Prof. Dr. Bernd Rech
Scientific Director

Prof. Dr. Jan Lüning
Scientific Director

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PROGRAMME

12th BESSY@HZB User Meeting on Thursday, December 10th 2020		
08:00 - 09:15	REGISTRATION & MATCH MAKING EVENT	75 Min.
09:15 - 10:20	**SYNCHROTRON SESSION (Chair: Christian Jung)**	65 Min.
09:15 - 09:20	Bernd Rech - Welcome to the User Meeting 2020	05 Min.
09:20 - 09:40	Jan Lüning - BESSY II Photon Science	20 Min.
09:40 - 10:00	Andreas Jankowiak - Accelerator Operation, Development and Projects	20 Min.
10:00 - 10:10	Antje Vollmer - Corona Measures at HZB	10 Min.
10:10 - 10:20	General Questions	10 Min.
10:20 - 11:00	BREAK: Vendor Exhibition & Poster Exhibition	40 Min.
11:00 - 11:40	**SCIENTIFIC LECTURES - PART I (Chair: Annette Pietzsch)**	40 Min.
11:00 - 11:20	Life Science & Health - Christian Feiler (HZB) HZB activities discovering new chemical entities to inhibit Sars-CoV-2 activity	20 Min.
11:20 - 11:40	Energy Storage - Sun Fu (QIBBT) Investigation of the decaying mechanism of solid state Li(Na) batteries by synchrotron X-ray tomography	20 Min.
11:40 - 12:00	BREAK: Vendor Exhibition & Poster Exhibition	20 Min.
12:00 - 13:00	**SCIENTIFIC LECTURES - PART II (Chair: Annette Pietzsch)**	60 Min.
12:00 - 12:20	Matter & Material - Rebecka Lindblad (Uppsala University) NEXAFS on small molecular ions	20 Min.
12:20 - 12:40	Information Technology - Yoav William Windsor (FHI) Deterministic control of an antiferromagnetic spin arrangement using ultrafast optical excitation	20 Min.
12:40 - 13:00	Energy Conversion - Ian Sharp (TU München) Advancing Solar Fuels Systems by Application of in situ Photoemission Spectroscopy to Active Solid/Liquid Interfaces	20 Min.
13:00 - 14:00	BREAK: Vendor Exhibition & Poster Exhibition	60 Min.
14:00 - 14:30	**POSTER SLAM (Chair: Roland Müller)**	30 Min.
14:30 - 15:30	**POSTER SESSION**	60 Min.
15:30 - 16:00	BREAK: Vendor Exhibition & Poster Exhibition	30 Min.
16:00 - 17:00	**Bestowal of Prices: Friends of Helmholtz-Zentrum Berlin e.V.**	60 Min.
17:00 - 17:30	BREAK: Vendor Exhibition & Poster Exhibition	30 Min.
17:30 - 18:30	**PUBLIC LECTURE - Rolf Hilgenfeld (Chair: Manfred Weiss)** Structure-based discovery of inhibitors of the SARS-CoV-2 main protease	60 Min.
ALL-DAY ALONGSIDE THE MEETING: VENDOR EXHIBITION & POSTER EXHIBITION		

ABSTRACTS OF THE SCIENTIFIC LECTURES

SCIENTIFIC TOPICS

Life Science & Health

Energy Storage

Matter & Material

Information Technology

Energy Conversion

Public Lecture

HZB activities discovering new chemical entities to inhibit Sars-CoV-2 activity

Christian Feiler

Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Right now, the world is plagued by the rampant COVID-19 pandemic. This pandemic leads to extensive human health concerns and is the cause of the global socio-economic disruption. Its causes are the severe acute respiratory syndrome coronavirus 2 (Sars-CoV-2). The virus, identified in December 2019 in Wuhan (China), spread rapidly worldwide. On January 30, 2020, the World Health Organization (WHO) identified the outbreak as a Public Health Emergency of International Concern and elevated the threat level to a global pandemic on March 11, 2020. The new virus, SARS-CoV2, caused more than 1.3 million deaths to date worldwide and more than 54 million infections (Nov., 14th 2020). Scientists worldwide conduct joint research to identify a vaccine or determine an antiviral drug treatment. The facilities for macromolecular crystallography at the Helmholtz-Zentrum Berlin (HZB) contributed to different approaches. Scientists at HZB utilized the well-established fragment screening workflow for drug discovery projects or are screening large compound libraries toward drug-repurposing attempts. HZB scientists founded a broad international scientific network spanning across Europe. All equal partners commit to the common goal with their scientific expertise. It is not the individual success that drives this collaborative approach, but the shared interest in contributing to the better.

References:

Dong, E (2020). The Lancet Infectious Diseases. 20, 533–534.

Drayman, Nir et al., bioRxiv: (2020) 08.31.274639. 1 Sep. 2020, preprint

Zhang, L., et al. (2020). Science. 368, 409–412.

Chen, J., et al. (2020). Journal of Molecular Biology. 432, 5212–5226

Zhou, P., et al. (2020). Nature. 579, 270–273

Weisberg, E., et al. (2020). Pharm. Res. 37, 167

Wollenhaupt J., et al., (2020) Structure. 28, 694-706.e5

Investigation of the decaying mechanisms of solid state Li(Na) batteries by synchrotron X-ray tomography

Fu Sun[1], Léo Duchêne[2], Ingo Manke[3]

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2 Empa, Swiss Federal Laboratories for Materials Science and Technology, CH-8600, Dübendorf, Switzerland
3 Institute of Applied Materials Helmholtz-Zentrum Berlin für Materialien und Energie Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Alkali metal-based all-solid-state batteries (ASSBs) promise to offer improved energy density, enhanced operational safety, and more flexible cell geometry (e.g., bipolar stacking) compared to the liquid battery counterparts[1]. They are considered one of the most crucial next-generation rechargeable battery technologies for electrochemical energy storage. Large scale research funding in both academy and industry around the world has been dedicated to this technology aiming to accelerate its transformation from laboratory research to practical commercialization. Despite these intensive research endeavours, the electrochemical performance of most laboratory prototype ASSBs remains unsatisfactorily poor even some of them are built with the new solid electrolytes (SEs) whose ionic conductivity surpass those of their conventional liquid electrolyte counterparts[2]. This indicates a significant knowledge gap in the understanding toward the underlying cause(s) for their performance decay during electrochemical cycling.

To gain fundamental insight into the mechanisms that govern the performance decay of ASSBs, herein, non-destructive synchrotron X-ray tomography technique is employed to directly visualize the electrochemically decayed Li and Na ASSBs without cell disassembly. The Li ASSBs were assembled with the sulfide superionic conductor $Li_{10}SnP_2S_{12}$ SE and the Na ASSBs were assembled with the $Na_4(B_{12}H_{12})(B_{10}H_{10})$ closo-borate SE. It is discovered that the main decaying mechanism for the Li ASSBs assembled with the sulfide SE is the side reaction between the SE and Li metal. In comparison, the main decaying mechanism for the Na ASSBs assembled with the closo-borate SE seems to be caused by an electrochemically inactive Na layer generated during the the battery cycling. These experimental results broaden the fundamental understanding of the degradation mechanisms of ASSBs and opens new opportunities for future research to advance the development of ASSBs.

References:

1 Nature Review Materials 2, 16103 (2017)

2 ACS Energy Letters 5, 922 (2020)

NEXAFS of small molecular ions

R. Lindblad[1,2,3], L. Kjellsson[4,5], R.C. Couto[6], M. Timm[2], C. Bülow[2], V. Zamudio-Bayer[2], M. Kubin[2], M. Lundberg[3], B. von Issendorff[7], J.T. Lau[2,7], S.L. Sorensen[1], J. Söderström[4], V. Carravetta[8], H. Ågren[4,6,9] and J.-E. Rubensson[4]

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3 Department of Chemistry-Ångström, Uppsala University, Sweden
4 Department of Physics and Astronomy, Uppsala University, Sweden
5 European XFEL, Germany
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7 Physikalishes Institut, Albert-Ludwigs-Universität Freiburg, Germany
8 IPCF-CNR, Pisa, Italy
9 Tomsk State University, Russia

The knowledge that can be obtained from NEXAFS measurements of small molecular cations adds to the current understanding of fundamental molecular physics. Compared to the neutral molecule, the cationic initial state has an additional valence vacancy. The core-excitation that takes place in NEXAFS of the molecular cation can therefore be compared to core-level XPS including shake-up states of the neutral molecule. But where the interpretation of XPS is complicated by overlapping final states, the dipole selection rules in NEXAFS simplifies the spectral interpretation. This allows experimental determination of spectroscopic constants of states, for which this has been regarded unfeasible using x-ray photoelectron spectra.

In this talk I will present NEXAFS measurements of the small molecular cations N_2^+, CO^+, N_2H^+ and NO^+ at the nitrogen or carbon and, when applicable, oxygen K-edges. The measurements have been performed at the Nano Cluster Trap end station at beamline UE52-PGM at BESSY II. Experimental results are compared to and analyzed by *ab initio* electron correlated wave function calculations.

References:

PRL 124, 203001 (2020)

PCCP 22, 16215-16223 (2020)

Deterministic control of an antiferromagnetic spin arrangement using ultrafast optical excitation

Y. W. Windsor[1], A. Ernst[2], K. Kummer[3], K. Kliemt[4], Ch. Schüßler-Langeheine[5], N. Pontius[5], U. Staub[6], E. V. Chulkov[7], C. Krellner[4], D. V. Vyalikh[7,8,] L. Rettig[1]

1 Fritz Haber Institute of the Max Planck Society, Germany
2 Johannes Kepler University, Austria
3 ESRF - The European Synchrotron, France
4 Johann Wolfgang Goethe-Universität, Germany
5 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
6 Paul Scherrer Institut, Switzerland
7 Donostia International Physics Center (DIPC), Spain
8 IKERBASQUE, Basque Foundation for Science, Spain

A central prospect of antiferromagnetic spintronics is to exploit magnetic properties that are unavailable with ferromagnets. However, this poses the challenge of accessing such properties for readout and control. To this end, light-induced manipulation of the transient ground state, e.g. by changing the magnetic anisotropy potential, opens promising pathways towards ultrafast deterministic control of antiferromagnetism. Here, we use this approach to trigger a coherent rotation of the entire long-range antiferromagnetic spin arrangement about a crystalline axis in $GdRh_2Si_2$ and demonstrate deterministic control of this rotation. Our observations can be explained by a laser-induced shift of the direction of the Gd spins' local magnetic anisotropy, and allow for a quantitative description of the transient magnetic anisotropy potential.

Reference:

Windsor et al, Communications Physics 3, 139 (2020)

Advancing Solar Fuels Systems by Application of *in situ* Photoemission Spectroscopy to Active Solid/Liquid Interfaces

Ian D. Sharp[1], Johanna Eichhorn[1], Marco Favaro[2], David Starr[2]

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2 Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institute for Solar Fuels, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The capture of solar energy and its direct conversion to chemical fuels in artificial photosystems provides a promising route to sustainably meet global energy demands and to overcome our current reliance on fossil fuels. However, development of practical photosystems has been impeded by a lack of semiconductor light absorbers that are simultaneously efficient and stable under the reactive conditions required for driving desired chemical reactions. To address this gap, elucidation of chemical transformations at active semiconductor/catalyst/electrolyte interfaces is urgently required. Fortunately, modern advances in ambient pressure X-ray photoelectron spectroscopy (AP-XPS) allow *in situ* characterization of electrified and illuminated photoelectrodes, thereby providing a route to improved understanding of catalytic mechanisms, (photo)corrosion pathways, and self-passivation reactions. Here, a brief overview of the major challenges in the realization of efficient and durable artificial photosynthesis devices, as well as the opportunities afforded by *in situ* "dip-and-pull" photoemission experiments at the newly commissioned BElChem endstation at BESSY-II, will be presented. In a first case example of the method, *in situ* photoemission experiments on multi-functional CoO_x coatings will be presented. These measurements reveal a critical role of biphasic materials for simultaneously promoting high catalytic activity and enhancing stability of Si electrodes. In a second example, recently performed measurements at the BElChem endstation on advanced Ta_3N_5 photoanodes under various bias and illumination conditions will be discussed. These experiments reveal complex interfacial reactions that involve formation of self-passivating surface layers with bias-dependent chemical properties. Illumination of the electrode at the open circuit potential in the presence of an Fe-based redox couple leads to formation of an ultrathin Fe oxide that improves both performance and stability. Together, these examples highlight the significant opportunities for advancing understanding of electrochemical and photoelectrochemical interfaces using *in situ* synchrotron-based X-ray photoelectron spectroscopy applied to solid/liquid interfaces.

PUBLIC LECTURE *17:30 - 18:30*

Structure-based discovery of inhibitors of the SARS-CoV-2 main protease"

Rolf Hilgenfeld

University of Lübeck, Institute of Molecular Medicine, Ratzeburger Allee 160, 23562 Lübeck, Germany

The RNA genome of the novel coronavirus SARS-CoV-2 codes for two cysteine proteases. The prime drug target among these is the main protease (also called 3CL protease), whereas the papain-like protease has a less favorable druggability profile. We have determined the crystal structure of the SARS-CoV-2 main protease using synchrotron radiation within 3 weeks of the publication of the genome of the new virus and used this structure to improve our pre-existing alpha-ketoamide inhibitors. In addition to peptidomimetics, we will discuss alternative approaches such as virtual screening, drug repurposing, and fragment-based drug discovery.

Reference:

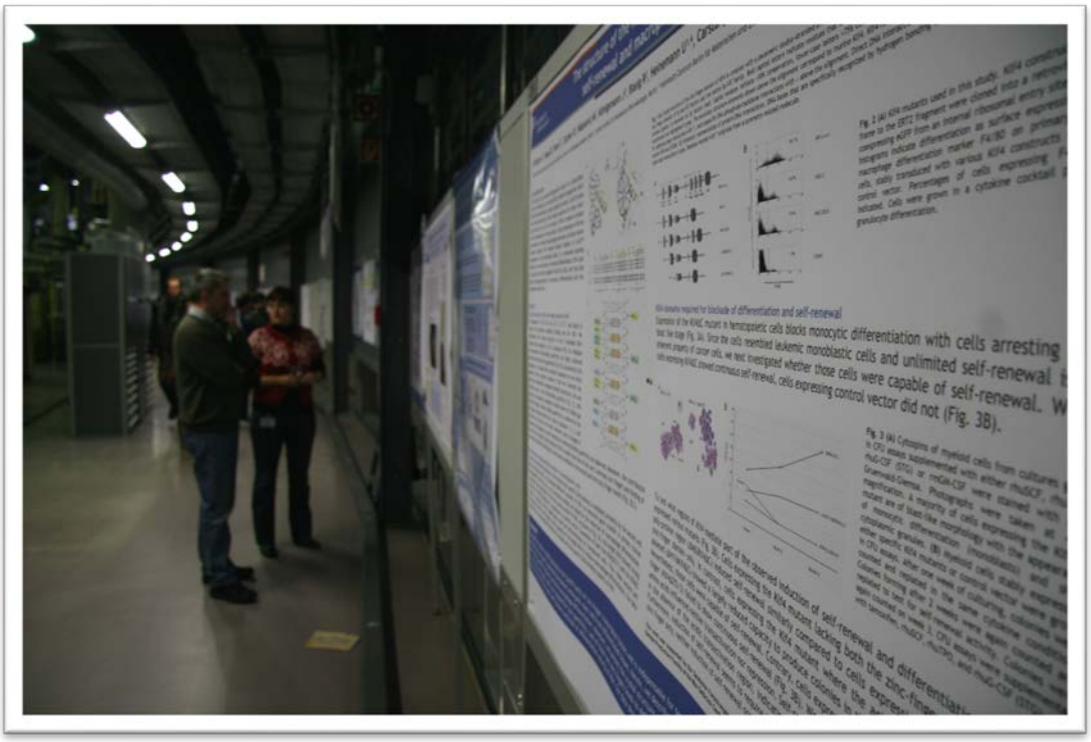
Zhang et al., Science 368, 409-412 (2020)

PLEASE NOTE

The Public Lecture will be streamed on the HZB YouTube channel

https://www.youtube.com/user/hzbKanal

This lecture is open to the general public, an access code is not required.



SCIENTIFIC TOPICS

Energy Conversion

Energy Storage

Information Technology

Life Science & Health

Matter & Material

Other

PTB Laboratory at BESSY II

In situ X-ray Analytics and Electrochemical Characterization Illuminate Nanoparticle Exsolution of Ni-doped Sr(Ti,Fe)O3-δ SOFC Electrode

Mauricio Arce (Helmholtz-Zentrum Berlin, Germany) *BElChem-PGM*

The mechanism of Fe-Ni nanoparticle exsolution from Ni-doped Sr(Ti,Fe)O3-δ for solid oxide fuel cells (SOFC) is studied using electrochemical impedance spectroscopy and synchrotron-based near ambient pressure X-ray photoelectron and absorption spectroscopies while redox-cycling. Understanding and control of the exsolution is key to lowering SOFC operation temperature.

Interface defects control photon upconversion performance in thin film halide perovskite-sensitized triplet-triplet annihilators

Karunanantharajah Prashanthan (Helmholtz-Zentrum Berlin, Germany) *HySPRINT*

Photon upconversion (UC) turns low-energy light into higher-energy light. We used thin film halide perovskite as triplet sensitizer for a triplet-triplet annihilation UC system. The carrier lifetime was correlated with UC efficiency. A 10-fold increase in UC efficiency was linked to a 6-fold increase in lifetime. We ascribe this to a processing-induced reduction in defects at the perovskite interface.

The Pt/Phosphoric Acid Interaction in HTPEMFCs: From the X-ray Spectroscopic Analysis of Reference Compounds to Operando Studies

Enggar Pramanto Wibowo (Helmholtz-Zentrum Berlin, Germany) *KMC-1*

To enhance the performance of high-temperature polymer electrolyte membrane fuel cells (HTPEMFCs), the elucidation of the interaction between the Pt catalyst and the phosphoric acid electrolyte is imperative. Detailed characterization of reference compounds by complementary x-ray spectroscopies paves the way for the study of the Pt/phosphoric acid interface under operating conditions.

Cation distribution in $Cu_2ZnSiSe_4$ from neutron diffraction and MEAD

Galina Gurieva (Helmholtz-Zentrum Berlin, Germany) *KMC-2*

The crystal structure of the $Cu_2ZnSiSe_4$ was studied using neutron diffraction (performed at FIREPOD at BER II) and suggested the presence of Cu/Zn disorder in this compound, previously considered to adopt orthorhombic wurtz-stannite structure. Subsequent MEAD study (performed at KMC-2 beamline at BESSY II) confirmed that $Cu_2ZnSiSe_4$ adopts monoclinic, wurtz-kesterite structure.

EXAFS investigation of anharmonic movements in chlorine substituted MAPbI3

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

Based on temperature-dependent Pb L3-edge EXAFS signals of chlorine-substituted MAPbI3 measured at the experimental station KMC-2 XANES, the anharmonic movements of the lead-halide bond were investigated in a temperature range from 20 K to 265 K. The temperature-dependence of the asymmetry of the distance distribution C3 and of the perpendicular Mean Square Relative Displacement will be discussed.

MEAD and cation distribution in CZTSe, CFTS, and CZSiSe

Daniel Többens (Helmholtz-Zentrum Berlin, Germany) *KMC-2*

Multiple Edge Anomalous Diffraction (MEAD) has been applied to various quaternary sulfide semiconductors in order to validate the distribution of Cu(I), Zn(II), and Fe(II) in the crystal structure. Beamline KMC-2 has been upgraded to allow tracking the intensity of selected Bragg peaks over an absorption edge by direct control of the monochromator from the diffraction endstation.

Influence of cation substitution on $BiFeO_3$ thin films on phase purity and optoelectronic properties

Pamela Machado da Silva Rattín (Institut de CIència de Materials de Barcelona, Spain) *KMC-3*

Cation engineering in ferroelectric $BiFeO_3$ thin films offers huge potential for photovoltaic applications. In this study, we present a thorough study on the influence of dopant composition and distribution on the structure, electronic and optical properties by means of high-resolution X-ray diffraction (KMC-3), X-ray absorption spectroscopy and spectroscopic ellipsometry.

Chemical and electronic structure of the Zn(O,S)/CIS interface as derived by photoelectron spectroscopy

Jakob Bombsch (Helmholtz-Zentrum Berlin, Germany) *UE48_EMIL*

$CuInS_2$ has been extensively studied as thin-film solar cell absorber. Discontinuity in the conduction band at the emitter/absorber interface has been discussed as one reason for the limited power conversion efficiency. Using direct and inverse photoelectron spectroscopy, we find an almost ideal energy level alignment at the Zn(O,S)/$CuInS_2$ heterojunction, principally allowing for high efficiencies.

Ir-Ti interaction in active and stable OER catalysts

Marianne van der Merwe (Helmholtz-Zentrum Berlin, Germany) *UE48_EMIL*

Titania-supported iridium oxide-based anodes are commonly used in PEM water electrolysis thanks to their excellent Oxygen Evolution Reaction (OER) performance. Yet, how the Ir-Ti ratio influences the OER activity and stability is not well understood. A combination of synchrotron-based X-ray analytics is used to examine the chemical and electronic structure of an Ir-Ti material library.

Model oxide perovskite electrocatalyst surfaces for water electrolysis

Christoph Baeumer (University of Twente, The Netherlands) *UE56-1_SGM*

Electrocatalysts are needed to store sustainable energy. Further advances rely on structure-activity relationships as derived from single crystalline surfaces. We demonstrate surface-composition-activity relationships in epitaxial $LaNiO_3$ thin films for water electrolysis. PEEM and spectroscopic investigation reveal how to tune the transformation pathways to a catalytically active surface phase.

Anoscopic surface decomposition of PBCO perovskite turns performance descriptors ambiguous

David N. Mueller (Forschungszentrum Jülich, Germany) *UE56-1_SGM*

The perovskite oxide (Pr,Ba)CoO_3 is shown to undergo nanoscale surface decomopsition after mere hours of exposure to application temperatures which could be resolved by X-Ray PEEM. Principal component and cluster analyis of the data suggests a Cahn-Hillard type decomposition which causes spatial inhomogeneieties in the electronic structure used as an activity descriptor, giving rise to ambiguitiy

Insights into the formation and composition of the SEI on carbon-coated TiO2 electrodes for Na-ion batteries by depth-dependent X-ray photoelectron spectroscopy

Andreas Siebert (Helmholtz-Zentrum Berlin, Germany) *KMC-1*

The chemical composition of the solid electrolyte interphase (SEI) on a TiO2 nanoparticle-based anode for sodium ion batteries was investigated by depth-dependent hard X-ray photoelectron spectroscopy (HAXPES) measurements, revealing the formation of a hydrocarbon layer at the electrode surface and a likely related downward bending of the anode energy levels at the interface with the SEI.

Spectroscopic Investigation of Silver Alloyed Cu(In,Ga)Se_2 Thin Film Solar Cell Absorbers

Donald Valenta (Helmholtz-Zentrum Berlin, Germany) *KMC-1*

Cu(In,Ga)Se_2 chalcopyrite thin films are widely used in photovoltaic cells. Silver-alloying to produce (Ag,Cu)(In,Ga)Se_2 can improve the opto-electronic properties, reduce structural defects, and can potentially enhance device performance. We use x-ray spectroscopy to get insights into the chemical and electronic structure in the surface and near-surface regions to relate to device properties.

In search of the reversible phase(s) in $Mg(BH_4)_2$

Rashmi Dahal (University of Stavanger, Norway) *RGBL Dipole*

SR-FTIR and XAS at B K-edge were used to study decomposition phases of $Mg(BH_4)_2$. The reaction steps were isolated with the help of thermogravimetric analysis combined with the differentiation scanning calorimetry. The results of the data analysis can shed light on the decomposition products of $Mg(BH_4)_2$ and thus indicate the pathways for improving the hydrogen storage properties of this compound.

Effective mass enhancement and ultrafast electron dynamics of Au(111) surface state coupled to a quantum well

Friedrich Freyse (Helmholtz-Zentrum Berlin, Germany) ***U125-2_RGBL***

The equilibrium band dispersion of the surface state of Au(111) quantum films grown on W(110) does not deviate from the expected free-electron-like behavior, its nonequilibrium energy-momentum dispersion probed by tr-ARPES exhibits a remarkable kink above the Fermi level. The kink is pronounced for certain thicknesses of the Au quantum well and vanishes in the very thin limit.

Ferromagnetic $MnSb_2Te_4$: A topological insulator with magnetic gap closing at high Curie temperatures of 45-50 K

Oliver Rader (Helmholtz-Zentrum Berlin, Germany) ***U125-2_RGBL***

Ferromagnetic $MnSb_2Te_4$: A topological insulator with magnetic gap closing at high Curie temperatures of 45-50 K Poster Abstract (max. 400 characters, no special characters): We show that p-type $MnSb_2Te_4$, previously considered trivial and antiferromagnetic is a ferromagnetic topological insulator with high Tc of 45-50 K as shown by spin-ARPES. It exhibits in STS a magnetically induced band gap that closes at the Curie temperature. Magnetic and structural disorder play an important role for the properties of this promising quantum anomalous Hall systems.

Atomic and electronic structure of a multidomain GeTe crystal

Jaime Sánchez-Barriga (Helmholtz-Zentrum Berlin, Germany) ***U125-2_RGBL***

We investigate the atomic and electronic properties of GeTe single crystals possessing a multidomain structure with inverted ferroelectric domains of 10-100 nm lateral dimensions. Using spin-ARPES, we establish a direct relationship between the opposite configurations of the ferroelectric polarization and a reversal of the Rashba-type spin texture of pure bulk states within individual nanodomains.

HMC hub matter - a resource for scientific data in Helmholtz

Oonagh Mannix (Helmholtz-Zentrum Berlin, Germany)

HMC hub matter is part of the new Helmholtz Metadata Collaboration, one of the Helmholtz incubator platforms. The hub aims to promote the qualitative enrichment of research data by means of metadata, thereby enhancing FAIRness of data. We present an example of how synchrotron tomography data can be connected with sample information, detailed experimental protocols, and a final journal publication

ExPaNDS - The benefits of Open Data

Kat Roarty (Diamond Light Source, United Kingdom)

ExPaNDS's will make the majority of PaN RIs data 'open' following the FAIR principles (Findable, Accessible, Interoperable, Reusable) according to the user's needs, and to harmonise efforts to migrate facility's data analysis workflows to EOSC platforms enabling them to be shared in a uniform way.

Self-Degrading Graphene Sheets for Tumor Therapy

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

Low biodegradability of graphene derivatives and related health risks are the main limiting factors for their in vivo biomedical applications. Here, we present the synthesis of enzyme-functionalized graphene sheets with self-degrading properties and their applications in tumor therapy. Due to their unique properties, the novel two-dimensional nanoplatforms can be used for anti-tumor applications.

Modulating the spliceosome with small molecules

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

Small molecules can be utilized to modulate protein-protein-interactions (PPIs) in large protein complexes like the spliceosome. Such modulation facilitates detailed analysis of the mRNA splicing process. Here, an essential spliceosomal PPI between Aar2 and Prp8 was targeted via crystallographic fragment screening, which successfully yielded small molecule starting points for downstream design.

Crystal structures of a bacterial transcriptional regulator RcdA in complexes with ligands

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

A transcriptional regulator RcdA belongs to TetR family. The first two effectors of RcdA, trimethylamine N-oxide (TMAO) and tris(hydroxymethyl)aminomethane (Tris), were identified indicating its potential role in alkaline stress response. Based on the obtained crystal structures of the RcdA-ligand complexes, the RcdA ligand-binding pocket was analyzed in details and described.

Beta-propeller lectin family from Photorhabdus laumondii

Eva Fujdiarova (Central European Institute of Technology Brno, Czech Republic) *MX Beamline*

We study atomic structures of lectins, sugar binding proteins, from a bacterium Photorhabdus laumondii. P. laumondii is living in mutualism with nematodes of the Heterorhabditis spp. This complex is highly pathogenic towards insect and is used as a biocontrol agents instead of pesticides. Studied lectins share a seven bladed beta-propeller fold and each of them have multiple sugar binding sites.

Structural ad Functional Analysis of the RNA Helicase HrpA

Lena Grass (Freie Universität Berlin, Germany) *MX Beamline*

RNA helicases are major players in post-transcriptional gene regulation. HrpA, a DExH-box helicase, boosts antibiotic tolerance in E.coli. Here, we present crystal structures of ecHrpA in an apo and RNA-bound conformation that reveal profound conformational changes. Structure-based functional analysis demonstrate how interfering with these distinct conformations directly effects protein activity.

baSHELiXir: phase fast, phase well!

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

We developed baSHELiXir for on-site evaluation experimental phasing data. We implemented several searches to determine previously unknown space group, solvent content, and high- or low-resolution limit. Procedures are parallelized. We wrote baSHELiXir to utilize the philosophy that ability to solve the phase problem is the best indication of useful anomalous signal in the experimental data.

Structure of unusual Inteins for Biotechnology Applications

Daniel Kümmel (Westfälische Wilhelms-Universität Münster, Germany) ***MX Beamline***

Inteins are powerful tools for biotechnological applications. Split intein fragments reconstitute into autocatalytic domains and can be used to fuse protein fragments or introduce labels. We have determined the structure of the intein TP105 that can be used for protein splicing applications under oxidizing conditions. The structures will be used to improve the intein by protein engineering.

Low dose measurements for spatially resolved anomalous dispersion refinement

Frank Lennartz (Humboldt-Universität zu Berlin, Germany) ***MX Beamline***

Spatially resolved anomalous dispersion (SpReAD) refinement is a mtehod that allows analysis of the oxidation states of individual protein-bound metals. Here, we have conducted such experiments on MX beamline 14.1. We have tested different transmission settings to vary the total dose per experiment and test whether data collected at low transmission are suitable for SpReAD refinement.

PAIREF - optimal cutoff with automated paired refinement

Martin Maly (Czech Technical University, Czech Republic) ***MX Beamline***

Where to cut the diffraction data from MX? Our recently released program PAIREF (pairef.fjfi.cvut.cz) provides automation of the paired refinement protocol - the current standard for determination of the optimal high-resolution cutoff. The procedure enables a direct linking of the quality of data and structure model that leads to coordinates closest to the truth.

Structural determination of plant phytochromes

Soshichiro Nagano (Justus-Liebig-Universität Giessen, Germany) ***MX Beamline***

Phytochromes are photoreceptor that regulate physiological activities in response to light in plants and other organisms. Phytochromes are photochromic, their activity being modulated by photoreversible conversion between red- and NIR-light absorbing states. We are using X-ray crystallography to understand plant phytochrome action at the molecular level. Here we describe the techniques we employ.

Dynamin as a Target for Structure-Based Fragment Screening

Helena Taberman (Helmholtz-Zentrum Berlin, Germany) ***MX Beamline***

Dynamin is a multidomain GTPase working in the endocytic pathway. It forms an oligomer around the neck of the invaginating vesicle, and the binding and hydrolysis of GTP introduces conformational changes inducing membrane fission. The HZB fragment screening workflow is used for finding novel small organic molecules binding to the different domains of dynamin for further drug development studies.

Structural Characterisation of Iodothyronine Deiodinases

Holly Towell (Universität Bayreuth, Germany) ***MX Beamline***

Iodothyronine deiodinases (Dio 1-3) are a family of selenocysteine-dependent enzymes that regulate thyroid hormone levels with differing regiospecificity. Solved monomeric structures of Dio2 & 3 are highly similar but reveal isoform specific loops. As the enzymes are homodimeric, a dimer structure would be useful to further understand the dimerization interface and the interaction with substrates.

Fragment screening via MX – starting points for drug design

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

HZB MX provides an efficient workflow for crystallographic fragment screening. It includes specialized fragment libraries, crystal handling tools, state-of-the-art beamlines as well as largely automated data analysis pipelines. The discovered hits present attractive starting points for structure-based ligand design. We support first steps of such designs based on commercially available compounds.

Exploiting the complementarity between X-ray Scattering and Absorption techniques to investigate breast cancer metastasis

Andre Conceição (Deutsches Elektronen-Synchrotron DESY, Germany) ***mySpot Beamline***

Accumulation of trace elements and its relationship with the matrix of the tumor microenvironment play an important role in supporting the growth and breast tumor progression. XRF was used to detected Fe, Cu and Zn, while the Rayleigh-to-Compton ratio technique (R/C) to access the light elements of the tissue matrix as well as SAXS to extract structural information of the tumor microenvironment.

How Hydrogen Bonding Amplifies Isomeric Differences in Pyridones Towards Strong Changes in Acidity and Tautomerism

Robby Büchner (Helmholtz-Zentrum Berlin) ***UE52_SGM***

The N K-edge NEXAFS of all Pyridone isomers in combination with molecular dynamics simulations connected to CASSCF and TD-DFT calculations yield the principles of Hydroxypyridine/Pyridone tautomersim and acidity: Steric hindrance of hydration and hydrogen bond enhancement by localized charges are the key factors for the massive differences between the isomers in aqueous solution.

Binding of β-lactam antibiotics by equine and ovine serum albumins

Kajetan Duszynski (Lodz University of Technology, Poland)

Serum albumins exhibit the remarkable ability of ligands binding. A number of these ligands are drugs, thus establishing the interactions of albumin-drug complexes is vital for understanding the pharmacokinetics. Until now, serum albumin-antibiotics structures are not known. We have determined first crystal structures of equine and ovine serum albumins in complexes with ß-lactam antibiotics.

An aspartic acid cluster in the reovirus attachment fiber acts as a pH-dependent molecular switch controlling trimerization

Giulia Glorani (Freie Universität Berlin, Germany)

During infection, the reovirus attachment protein sigma1, undergoes conformational changes, triggered by environmental pH. Thermostability and oligomeric state of sigma1 WT and mutants were analyzed at different pHs, identifying the Asp-345 as an attractive candidate for a molecular switch and as a requirement for the stability of the trimeric sigma1, especially in a low to neutral pH environment.

The tetrameric structure of a novel haloalkane dehalogenase

Andrii Mazur (University of South Bohemia, Czech Republic)

The novel haloalkane dehalogenase DpaA was isolated from the Paraglaciecola agarilytica NO2. The DpaA enzyme was crystallized using the sitting drop vapour diffusion method, yielding crystals that diffracted X-rays to 2.0 Å resolution. Diffraction data analysis resulted in a tetrameric model of DpaA, highlighting an uncommon multimeric nature for a protein belonging to the HLD-I subfamily.

X-Ray Fluorescence Imaging with Coded Apertures

Anicó Kulow (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

X-ray fluorescence (XRF) imaging is a powerful tool for the investigation of the elemental distribution in materials. We developed a method for full-field XRF imaging based on coded apertures, consisting of multiple pinholes arranged in a known pattern that produce overlapping projections on the detector. For the retrieval of the object information we developed different reconstruction algorithms.

Evolution of CFRP stress cracks observed by in-situ X-ray refractive imaging

Andreas Kupsch (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

We report on in-situ synchrotron X-ray imaging of tensile stress induced cracks in carbon fiber reinforced plastics due to inter-fiber failure. A compact tensile testing machine with a load range up to 15 kN was integrated into Diffraction Enhanced Imaging (DEI) set-up of the BAMline. DEI allows to observe the evolution of cracks in large fields-of-view at sufficient image contrast.

Synchrotron X-Ray Tomography Techniques at BAMline

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

Synchrotron X-Ray computed tomography at the BAMline is constantly evolving. During monochromatic tomographic scans a preview reconstruction is offered. Newly introduced scanning schemes suppress certain types of reconstruction artifacts. Additionally, the application of a pink beam enables for faster tomographic scans within minutes.

Local probe of single-phase fcc-structured $Al_{0.3}$-FeCoNiCr HEA

Alevtina Smekhova (Helmholtz-Zentrum Berlin, Germany) ***BAMline, PM2-VEKMAG, UE46_PGM-1***

XAS/XMCD techniques have been applied to probe the local environment, electronic structure and magnetic moments in as-cast fcc-structured single-phase Al0.3-FeCoNiCr high-entropy alloy. A homogeneous local coordination with only a surface oxidation of constituents was found. After in situ cleaning by Argon, Fe, Co and Ni atoms demonstrated a metallic character and reduced magnetic moments.

Experimental determination of differential scattering coefficients by means of linearly polarized X-ray radiation

André Wählisch (Physikalisch-Technische Bundesanstalt, Germany) ***BAMline***

By using the highly linear polarization characteristics of the synchrotron radiation available at BESSY II we determine polarized differential scattering cross sections for monochromatic excitation from non-resonant scattering experiments. This quantitative work is focused on accurately ascertaining the experimental uncertainty budget.

Room temperature unconventional charge ordering in tunnel ruthernate $Na_{2.7}Ru_4O_9$

Arvind Yogi (UGC-DAE Consortium for Scientific Research, India) *CoreLab CCMS (Microscopy)*

Charge degrees of freedom with spin-orbital coupling (SOC) is an interesting playground for emergent electronic phenomena. Our extensive TEM investigation explicitly unveils the CO and microscopic structural and spectroscopic nature of $Na_{2.7}Ru_4O_9$. The crystal field distortions induce high spin (HS) to low spin (LS) crossover in 4d4 Ru ion leading to first order transitions at Tc = 365 K-345 K.

Core Lab Quantum Materials

Konrad Siemensmeyer (Helmholtz-Zentrum Berlin, Germany) *CoreLab QM (Quantum Material)*

New material preparation in powder and single crystal form. Material analysis: stoichiometry, single crystallinity etc. Orientation, shaping and (multiple) mount of crystals Temperature, field and pressure dependence of magnetisation, resistivity, specific heat, thermal transport, Wide temperature range: 0.4 K – 1100 K, dependent on methods, magnetic field up to 14 Tesla, pressure cells available.

Investigating electronic structure and molecular orientation of extended aromatic molecules with NEXAFS

Daniel Bischof (Philipps-Universität Marburg, Germany) *HE-SGM*

The analysis of NEXAFS signatures of extended aromatic hydrocarbons provides information on the unoccupied electronic states, unveiling a unilaterally fluorinated acene derivative as a connecting link between its parental molecules. NEXAFS dichroism measurements can be utilized to determine the molecular orientation of organic semiconductors, revealing a strong dependence on the substrate quality.

Photo-aging of polybutylene succinate (PBS) biopolymer - Impact of UV-Vis exposure on surface weathering

Melanie Fritz (University Koblenz-Landau - Department of Physics, Germany) *HE-SGM*

Exposing polymers to UV-Vis radiation leads to significant degradation and leaching. This weathering cannot be prevented by photo stabilizers, thus changing surface properties. Polybutylene succinate (PBS) was photo-aged, characterized by contact angle and SEM, chemical composition determined by NEXAFS and XPS. The results showed differences in initial stages of aging for PBS.

Redox-switchable rotaxanes of gold surfaces

Mihkel Ilisson (Freie Universität Berlin, Germany) *HE-SGM*

Rotaxanes including a redox-switchable ring and terpyridine coordination site(s) will be synthesized and deposited to Au-surfaces. The surfaces will be analysed by different methods, including XPS and NEXAFS measurements at BESSY II to investigate deposition efficiency, regularity, surface structure as well as changes of the structure upon electrochemical switching.

Plasma functionalization and doping of graphene: NEXAFS vs. molecular dynamic simulations

Andrea Jagodar (GREMI University of Orléans, France) *HE-SGM*

In this work, we present an analysis of plasma functionalized/doped vertically aligned graphene nanowalls obtained by SEM, XPS, and NEXAFS spectroscopy. This analysis is compared with MD simulation revealing plasma surface activities.

Polymer synthesis by pulsed RF plasma

Eva Kovacevic (GREMI University of Orléans, France) *HE-SGM*

We present NEXAFS and XPS analysis of polymers synthesized by means of multipulse-modulated RF discharges. This type of discharges can be used for a production of nanostructures as well as for a deposition of smooth ultra-thin films interesting for various technological (industrial) applications.

X-ray spectroscopic analysis of thin plasma deposited amorphous carbon layers (a-C:H) on polyamide 6 (PA6): Determination of the interlayer thickness

Torben Schlebrowski (Universität Koblenz-Landau, Germany) *HE-SGM*

Polymers are often coated with an amorphous hydrogenated carbon layer (a-C:H) to adapt it to new applications. Their stability on the base material depends directly on the characteristics of an interlayer, a mixed region of polymer and a-C:H layer. Here X-ray spectroscopic measurements are presented to determine the thickness of the interlayer in a-C:H coated PA6 samples

PM-SIRMS: a pragmatic tool for polymer science and engineering

Stan Looijmans (Eindhoven University of Technology, The Netherlands) *IRIS*

PM-SIRMS: a pragmatic tool for polymer science and engineering Poster Abstract (max. 400 characters, no special characters): Polymer properties are determined by the microstructure. In semi-crystalline polymers the structure, morphology and molecular orientation are generally quantified using X-ray scattering and diffraction. A versatile technique based on infrared spectroscopy is emerging. By modulating the polarization of the incident light, local anisotropy can be studied in real time on a sub-molecular length scale.

FTIR microspectroscopy of plant cells

Victor Rodriguez Zancajo (Humboldt Universität zu Berlin, Germany) *IRIS*

Cell wall composition and structure govern functions such as seed propagation, mechanical support and stress resistance. Understanding function of plant tissues requires to elucidate the interaction of organic and inorganic materials. FTIR combined with multivariate techniques allows histological characterization of the tissues ranging from the micro-morphology to the molecular composition.

Etalon Effects in THz Film Measurements

Ulrich Schade (Helmholtz-Zentrum Berlin, Germany) *IRIS*

Etalon effects in THz transmittance spectra, either taken in time-domain or frequency-domain, often hamper or even hinder the interpretation of film properties. We discuss the transferability and applicability of spectroscopic methods typically employed in the near and mid infrared spectral range to eliminate the fringes in the transmittance spectra in the THz spectral range.

Flow Focused Droplet Train for APXPS

Pip Clark (Helmholtz-Zentrum Berlin, Germany) *KMC-1*

We designed a droplet train for measuring the chemical and physical properties of liquids in pressures up to 30 mbar with the SpAnTeX endstation. It generates thousands of uniform droplets a second, with diameters tuneable from 100 to 500 microns. We show commissioning experiments on aqueous solutions, colloidal systems, and demonstrate time-resolved capabilities with salt nucleation and growth.

Instrumentation for in situ PXRD on nanoporous crystalline materials upon applying of combination of stimuli

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

Soft porous crystals (SPC) attract considerable attention due to their unique properties and potential application in gas storage, separation and sensory technique. In the current contribution, we design unique instrumentation, which allow to follow the structural transition in SPCs by synchrotron PXRD upon applying the combination of stimuli such as gas molecules and UV light or electric field.

X-ray spectroscopic study of magnetic ferrite nanoparticles for theranostic applications: effect of size and distribution

Fani Pinakidou (Aristotle University of Thessaloniki, Greece) *KMC-2*

Micro-XRF mapping and Fe-K-XAFS measurements is applied in order to study the spatial distribution, bonding environment and valency of Fe in Fe_3O_4 nanoparticles of various sizes prior to and after hyperthermia. It is demonstrated that the distribution of the MNPs differs as a function of both size and hyperthermia while partial oxidation of Fe^{2+} species as well as modification in site occupancy is expected.

High resolution X-ray diffraction studies on porous silicon

Cosmin Romanitan (National Institute for R&D for Microtechnologies Bucharest, Romania) *KMC-2*

Porous silicon layers were obtained using the electrochemical etching of bulk Si at different current densities. As the result, porous layers with different morphologies were obtained. High resolution x-ray diffraction allowed us to get the lattice strain and the mean pore diameter, while x-ray reciprocal space mapping allowed us to get the mean porosity given by the whole volume of the samples.

Hybrid perovskite crystallization from binary solvent mixtures: interplay of evaporation rate and binding strength of solvents

Oleksandra Shargaieva (Helmholtz-Zentrum Berlin, Germany) ***KMC-2***

In this work, we rationalize the chemical pathways and kinetics of the crystallization of methylammonium lead iodide hybrid perovskite via analysis of solvent coordination, the structure of intermediate solvate phases, and modeling evaporation rates of precursor solutions. The evolution of solution species via intermediate solvate phases and into perovskite thin films was monitored by in-situ GIWAXS.

XPP-KMC-3: The time-resolved hard X-ray diffraction endstation at BESSY II

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

The XPP endstation installed at the KMC-3 beamline is dedicated to 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 observed ultrafast structural response using different excitation and detection schemes available at XPP KMC-3.

Grazing exit X-ray fluorescence (GEXRF) analysis of high entropy alloys (HEA) and compositionally complex alloys (CCA)

Cafer Tufan Cakir (Bundesanstalt für Materialforschung und -prüfung, Germany) ***mySpot Beamline***

Special attention has been drawn to HEAs and CCAs regarding their corrosion behavior. In order to investigate how HEAs and CCAs behave in corrosive environment, GEXRF provides notable information in the nanometer to micrometer range for the understanding of high temperature oxidation mechanisms.

Reversible switching between positive and negative thermal expansion in a metal-organic framework DUT-49

Volodymyr Bon (Technische Universität Dresden, Germany) ***MX Beamline***

Stimuli responsiveness of porous metal-organic frameworks (MOFs) has led to important inventions in the field of switchable materials. Herein, we present the first report for simultaneous positive and negative thermal expansion for the same MOF structure, under different conditions applied. A detailed study on the effect of guests for varying the flexibility of DUT-49 framework is also described.

SAXS CT reconstruction of a test object containing standard scattering samples

Christian Gollwitzer (Physikalisch-Technische Bundesanstalt, Germany) ***MX Beamline***

SAXS CT is a method where the small-angle X-ray scattering signal is measured for different angles and positions of the incident beam onto the sample. This allows the reconstruction of the inner structure of the sample, resulting in a SAXS signal for every voxel. We fabricated a test sample containing SAXS reference standards and successfully reconstructed the data taken at the MX 14.1 beamline.

Reflection zone plates on spherical substrates for flat field soft X-ray spectroscopy

Alexei Erko (Institut für angewandte Photonik e. V., Germany) *Optics Beamline*

First experimental results obtained with a soft X-ray spectrometer, based on reflection zone plates (RZPs) fabricated on a spherical substrate with a radius of 29.9 m, are described. High resolution parallel spectra were measured in the interval from 150 eV to 750 eV. The absolute diffraction efficiency reaches 25 %. The energy resolving power $E/\Delta E$ exceeds ~ 1000 in the entire energy range. An algorithm for diffractive wavefront correction was used for the calculation of the groove structure.

Charge transfer induced interfacial ferromagnetism in $La_{0.7}Sr_{0.3}MnO_3/NdNiO_3$

Kai Chen (Helmholtz-Zentrum Berlin, Germany) *PM2-VEKMAG*

Charge transfer induced interfacial ferromagnetism and its impact on the exchange bias effect in the correlated oxide heterostructures of $La_{0.7}Sr_{0.3}MnO_3/NdNiO_3$ are investigated by soft x-ray absorption and x-ray magnetic circular dichroism spectra from 10 to 300K. Besides the antiferromagnetic Ni^{3+} cations in the $NdNiO_3$ layer, Ni^{2+} ions are formed due to a charge transfer mechanism at the interface.

Observation of ferrimagnetic skyrmions in $DyCo_3$

Kai Chen (Helmholtz-Zentrum Berlin, Germany) *PM2-VEKMAG*

We report the observation of ferrimagnetic bubble skyrmions in $DyCo_3$ single layer. These skyrmions, with the antiparallel aligned Dy and Co magnetic moments and with characteristic lateral sizes of about 40 nm are formed during the nucleation and the annihilation of the magnetic maze-like domains with an obvious topological Hall effect.

Important role of uncompensated moments in noncollinear antiferromagnetic Mn_3Ir and Mn_3Sn epitaxial thin films

James Taylor (Helmholtz-Zentrum Berlin, Germany) *PM2-VEKMAG*

The noncollinear antiferromagnets Mn_3Ir and Mn_3Sn are of interest for topological spintronics. However, control of their triangular magnetic structure remains a challenge. In this poster, we explain how XMCD measurements have helped reveal the important role of uncompensated Mn moments in manipulating spin texture chirality in thin films of these materials.

Blocking and transition temperatures of light- and temperature-driven spin transition of adsorbed spin crossover molecules

Jorge Torres (Freie Universität Berlin, Germany) *PM2-VEKMAG*

Different coverages of two Fe(II) spin crossover molecules were deposited by thermal evaporation on a graphite substrate and their light- and temperature-induced transition between low spin (S = 0) and high spin (S = 2) investigated by x-ray absorption spectroscopy at the VEKMAG end station of PM-2. Results highlight the role of the molecular ligands for the stabilization of the high-spin state.

Signature of anisotropic exchange interaction revealed by vector-field control of helical order in an FeGe thin plate

Le Yu (École polytechnique fédérale de Lausanne, Switzerland) ***PM2-VEKMAG***

We used the unique vector-field setup at VEKMAG and resonant small-angle x-ray scattering on chiral magnet FeGe. The results show that the direction of helical propagation can be controlled by directional magnetic field training. The observed anisotropy in the helical modulation period is explained by the inclusion of higher-order anisotropic exchange in the Bak-Jensen model.

Stability of radical-functionalized gold surfaces

Tobias Junghöfer (Eberhard Karls Universität Tübingen, Germany) ***PM4***

We investigated the functionalization of gold surfaces with a derivative of the perchlortriphenylmethyl (PTM) radical using two related methods. We examined the resulting self-assembled monolayers using X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. The results show a system with the prerequisite stability for device application.

Eu^{3+} doped borosilicate glass after electron beam irradiation

Ekaterina Ivanova (Ioffe Institute, Russian Federation) ***RGBL Dipole***

Borosilicate glass, activated by Eu^{3+} ion, was studied. Electron beam irradiation with an energy of 20 keV lead to appearance of intense blue luminescence. It was found by electron probe microanalysis that the sodium content significantly decreases under electron beam irradiation. XPS studies shows change in atomic composition of sample surface and appearance of unidentified feature.

Thermal oxidation of molybdenium in air

Mikhail Lapushkin (Ioffe Institute, Russian Federation) ***RGBL Dipole***

Thermal oxidation of molybdenum in air has been studied. It is shown that a thick oxide film MoO_3 is formed. It was found that during the oxidation of molybdenum, dissociative adsorption of water molecules occurs.

Graphene functionalization: towards new materials' properties and applications

Maxim Rabchinskii (Ioffe Institute, Russian Federation) ***RGBL Dipole***

In this work, we present our results on a long-term study of the synthesis, study, and application of a set of functionalized graphenes. We demonstrate that the performed chemical modifications allow to rationally design the electronic structure and physics of the graphene layer, making advance within the field of its application within the field of sensing and nanocomposites manufacturing.

Coordination crosslinking of helical oligoamide nanorods: controlling independent SSA motifs

Norton West (La Trobe University, Australia) *THz-Beamline*

We have versatile tuneable one- to two-dimensional superstructures based on independent multi-tiered supramolecular self-assembly developed upon metal coordinated oligoamide nanorods. The peptide backbone is unaffected by metal coordination, as shown by FT-IR. XPS studies have shown that the Cu^{2+} ions were reduced to +1 and 0 oxidation states and were coordinated to the histidine and carboxylate.

PEAXIS - A High Resolution RIXS Endstation for Energy and Quantum Material

Deniz Wong (Helmholtz-Zentrum Berlin, Germany) *U41-PEAXIS*

Material systems for energy and quantum applications are accompanied with complex electronic structures. High resolution RIXS allows exploring the coupling of the material's lattice with its electronic structure. PEAXIS offers unique features that cater the needs of studying modern material systems with wide temperature range, applied voltage devices and continuous motion for sensitive samples.

High- resolution spectromicroscopy study of Si compounds in microchips at U41-PGM1-XM

Kristina Kutukova (Fraunhofer Institute for Ceramic Technologies and Systems, Germany) *U41-TXM*

Full-field microscopy at U41-TXM was combined with spectomicroscopy at x-sections of microchip. Si-K absorption spectra is indicating different types of dielectrics between Cu interconnects: porous OSG and SiCN, and N-K spectra is an existence of N in SiCN. The study demonstrates that spectromicroscopy allows to analyze patterned structures in microchip manufactured in 14 nm CMOS technology node.

Cation- and lattice-site-selective magnetic depth profiles of ultrathin Fe_3O_4(001) films

Karsten Küpper (Universität Osnabrück, Germany) *UE46_PGM-1*

XRMR is a technique combining the depth resolution of X-Ray Reflectivity and the site- and magnetism-sensitivity of XMCD. This enables us to determine the magnetooptical depth profiles of a Fe_3O_4 thin film at the energies characteristic for Fe^{2+}oct, Fe^{3+}tet, and Fe^{3+}oct in the XMCD. We find a ~3.9Å layer of enhanced magnetooptical absorption at the surface for both Fe^{3+} species but not for Fe^{2+}.

Testing High-throughput XPS analysis for Combinatorial Material Science, using a NiO-Cu2O Library

Lucas Bodenstein-Dresler (Helmholtz-Zentrum Berlin, Germany) *UE48_EMIL*

A 72 x 72 mm2 combinatorial library of NiO-Cu2O HTL candidate materials for solar cells was studied by XPS to look for composition-dependent surface chemical - electronic correlations. The data from a 13 x 13 grid of measurement points were evaluated by two approaches, viz. coarse, but fast, and detailed, but time-consuming, to test how suitable is the former for true high-throughput XPS analysis.

Nanoscale characterization of chemical and electronic structure of electrodeposited Cu-In-Se bulk homojunctions

Nina Novakovic-Marinkovic (Helmholtz-Zentrum Berlin, Germany) *UE49_PGM SPEEM*

We use PEEM to explore morphology and electronic properties of the nano pn bulk homojunctions (BHJ) of CuInSe (CISe) compounds. Single step electrodeposition creates self stabilized film of an interconnected 3D network of highly ordered, nanoscale pCISe/nCISe BHJs. We present the analysis of grain distribution on the sample surface and deduct from the work function how pn junctions are formed.

Quantification of Ni L2,3 core-hole relaxation pathways utilizing Auger-photoelectron coincidence spectroscopy

Artur Born (Helmholtz-Zentrum Berlin, Germany) *UE52_PGM CoESCA*

Ni LVV Auger spectra, in coincidence with the corresponding L2, L3 and 6eV satellite photoelectrons, have been used to examine electron correlation and itinerance effects in Ni.

Ultrafast X-ray spectroscopy reveals the role of the solvent in $Fe(CO)_5$ ligand substitution dynamics

Hampus Wikmark (Uppsala University, Sweden) *UE52_SGM*

We have studied the spin and charge aspects of ligand substitution for $Fe(CO)_5$ in three solvents, on the ns-ps scale, at the BESSY II facility using a liquid jet, pumped by a UV laser and probed by X-ray absorption spectroscopy at the Fe L absorption edge. The triplet-singlet complex conversion rate is much higher in ethanol, indicating the strong influence of the solvent nature on this process.

Directional charge mobility in semiconducting 2H-MoS_2 and metallic 1T-Li_xMoS_2

Robert Haverkamp (Helmholtz-Zentrum Berlin, Germany) *UE56-1_PGM*

By means of the core hole clock approach at the S L1 absorption edge we investigated the directional charge transfer for selectively prepared in-plane and out-of-plane electronic states on a sub-fs timescale in 2H-MoS_2 as well as 1T-Li_xMoS_2.

Complementary transient soft NEXAFS spectroscopy on thin films using lab equipment and synchrotron radiation

Ioanna Mantouvalou (Helmholtz-Zentrum Berlin, Germany) *UE56-1_PGM*

We present transient NEXAFS measurements on thin films using NEXAFS spectrometers at BLiX at the TU Berlin and compare the results to measurements at the UE56-1_PGM beamline. The thin films are measured in transmission mode and pumped optically using different time resolution and delays. The complementarity of the measurements is evaluated and new opportunities will be discussed.

Spin and orbital magnetic origin of stripe domains

Derang Cao (Forschungszentrum Jülich, Germany) ***UE56-1_SGM***

Stripe domain (SD) structure film owns the in-plane domain, out-of-plane domain, closure domain, Bloch and Néel wall. By using X-ray magnetic circular dichroism (XMCD) -based techniques, the existence of the various magnetization distribution in the film will show different XMCD signal strength. The contribution of local element-resolved spin and orbital magnetic moments of SD film can be determined.

mfCVD – Control over electronic structure of iron oxide thin films

Anja Sutorius (Universität zu Köln, Germany) ***UE56-1_SGM***

mf-CVD offers a direct pathway to manipulate the evolution of microstructure, phase composition, and magnetic properties of the prepared film. We report on the role of applied magnetic fields during a cold-wall CVD deposition of iron oxide from [FeIII(OtBu)3]2 leading to higher crystallinity, larger particulates, and better out-of-plane magnetic anisotropy, if compared with zero-field depositions.

Link of Ultra fast spin dynamics and magnetic domain structure

Fangzhou Wang (Forschungszentrum Jülich, Germany) ***UE56-1_SGM***

Explore the missing link between spin dynamics ultrafast laser-induced with accumulative all-optical domain formation in [Co/Pt]3 ferromagnetic multilayer system with perpendicular magnetization anisotropy. PEEM-XMCD images are measured at the Co L3 edge and the spatial structure of the magnetic domain is obtained with nm resolution.

Synthesis and characterization of neodymium doped TiO_2 nanoparticles and their application as nanothermometers

Selene Acosta (University of Mons, Belgium)

Neodymium doped TiO_2 nanoparticles were synthesized by the sol-gel technique and characterized via XRD, XPS, SEM, TEM, EDX and TXM-NEXAFS. Through the analysis of the M-edges recorded on single Nd-TiO_2 nanoparticles, the oxidation state of the dopant was evaluated. Lastly, Nd-TiO_2 nanoparticles were tested as nanothermometers due to their temperature dependent photoluminescence.

Novel Technique for On-Line Monitoring of the Curing Process of Fiber Reinforced Polymer Composites

Jörg Beckmann (Bundesanstalt für Materialforschung- und Prüfung, Germany)

The knowledge of the cure situation during the production process of the thermosetting material is of enormous importance. Mid- and near- infrared (IR) spectroscopy in attenuated total reflectance (ATR) geometry are promising techniques for curing studies. An IR/THz sensor system was developed to investigate its suitability for future online monitoring of curing processes in the production line.

The p(1×3)-O reconstructions on Mo(112) are actually imperfect forms of the p(2×3)-O

Teng Ma (Shenyang Agricultural University, China)

A critical precursor of the p(2x3)-O has been found during its stepwise formation process in O_2 by STM and XPS. It could not only give a reasonable explanation about the contraries between STM images and streaky LEED points, but also show the p(2x3)-O precursor is related to the p(1x3)-O reconstruction, which is actually the imperfect p(2x3)-O reconstruction. Furthermore, the imperfect p(2x3)-O observed as the p(1x3)-O has two different forms: an unfinished or the damaged one.

Electron and hole charge transport and traps in halide perovskites

Artem Musiienko (Helmholtz-Zentrum Berlin, Germany)

Several studies indicated the critical role of defects on the performance of perovskite devices. However, the parameters of defects and their interplay with free charge carriers remain unclear. Our results provide an insight on electron and hole transport properties of perovskite semiconductors.

Local spin canting, weak Jahn–Teller distortion, and magnetic compensation in $Ti_{1-x}Mn_xCo_2O_4$ spinel

Pramanik Prativa (Indian Institute of Technology Guwahati, India) ***BER II***

We present the evidence for Local spin canting, weak Jahn–Teller distortion (c/a < 1), and spin-compensation effect in $TiMnCo_2O_4$ spinel using the Neutron Diffraction Studies performed at HZB-BER-II. Ferrimagnetic (FiM) ordering sets in the system due to the presence of unequal magnetic moments of cations. Also an additional weak AFM component is noticed lying perpendicular to the FiM component.

Reentrant Spin-glass state from Neutron Scattering Study of few Complex Spinels

Thota Subhash (Indian Institute of Technology Guwahati, India) ***BER II***

We present the results of Neutron scattering studies on the Co_2TiO_4 single crystals using E2, E6, and E9 instruments available at HZB-BER II reactor. Reentrant spin-glass state below the ferrimagnetic ordering, diffusive character of (111) reflection and anisotropic local strain effects are observed due to competing Jahn-Teller effects acting along different crystallographic axes of the system.

OTHER TOPICS *BEAMLINE*

Polylactide acid (PLA) as base material for a-C:H films deposited in various angle geometries resulting in changed surface properties

Lucas Beucher (Universität Koblenz-Landau, Germany) ***HE-SGM***

The biodegradable polymer PLA is surface modified by plasma enhanced chemical vapor deposition with thin a-C:H films. Resulting properties depend on the sp2/sp3 ratio and H-content, which can be varied by angle-dependent coating, impacting chemical structure, contact angle and water vapor transmission rate. This expands the range of applications and enables customized functionalities.

C-amidation of substituted beta-3 oligoamides yields novel supramolecular assembly motif

Claire Buchanan (Latrobe University, Australia) ***IRIS***

Substituted beta-3 oligoamides form a unique 14-helix secondary structures via a 3-point H-bond motif of the amide backbone. N-acetylation creates a 3rd H-bond pair, extending this motif to intramolecular self-assembly. In this work, a new H-bond pair is created via C-terminal amidation. Analysis by AFM, SANS, and Far & Mid-IR shows that C-amidation promotes a unique supramolecular assembly motif.

Studying pigments from the legacy of A. Boecklin and E. Munch by synchrotron far-infrared spectroscopy

Hartmut Kutzke (Museum of Cultural History University of Oslo, Norway) ***IRIS***

Collections of pigments from the Swiss painter Arnold Böcklin and the Norwegian artist Edvard Munch were investigated by far infrared spectroscopy at the IRIS beamline. FIR provides Information on oxides and sulphides otherwise undetectable by MIR. This is first systematic FIR research on original artistic material, providing detailed analysis of components and any potential alteration products.

IRIS Microscopy station upgrade: Spatial, Temporal and Polarisation resolved spectroscopy

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

The IRIS microcopy station is upgraded through a BMBF project between the HU Berlin and the HZB. The set-up combines diffraction limited IR microscope with imaging and polarisation modulation, Raman, and scattering-type scanning near-field optical microscopes. This multimodal beamline set up provides chemical information which spans the spatial resolution from microns to tenths of nanometres.

A New Scanning Transmission X-ray Microscope At UE48/EMIL

Markus Weigand (Helmholtz-Zentrum Berlin, Germany) ***UE48_EMIL***

Scanning X-ray microscopes are a powerful tool for investigation of materials on the nanoscale, using x-ray absorption as an element, chemical and magnetically sensitive contrast mechanism via NEXAFS/XMCD. We will show an overview of a new state-of-the art custom build instrument that has recently been installed at the EMIL beamline and is planned to go in operation in the 2nd half of 2021.

Viewing RIXS experiment results with ADLER

Maciej Bartkowiak (Helmholtz-Zentrum Berlin, Germany) *U41-PEAXIS*

Several software tools are being developed as a part of the user program on the PEAXIS instrument at HZB. Here we demonstrate ADLER (Advanced Data Loading, Evaluation and Reduction), developed to simplify the visualisation and reduction of the Resonant Inelastic X-ray Scattering data.

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

Annick Froideval (Helmholtz-Zentrum Dresden-Rossendorf e.V., Germany)

The European Synchrotron and free-electron laser User Organisation (ESUO) represents about 22.000 users from 30 European member states and associated countries. Each country is represented within ESUO by one up to four national delegate(s), depending on the size of the user community in the respective country. The ESUO aims and activities are shown in this poster.

SyncLab – Combined X-ray methods at BLiX and BESSY II

Birgit Kanngießer (Technische Universität Berlin, Germany)

The new joint research group SyncLab between the TU Berlin and HZB evaluates the synergies of measurements using lab sources and synchrotron radiation. This is facilitated by the instrumentation at BLiX at the TU Berlin which is dedicated to the development of novel instrumentation and methodology for lab analysis. We present the new opportunities for HZB and external users offered by SyncLab

Photoemission from Liquid Jets: New Developments

Sebastian Malerz (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)

Photoelectron circular dichroism (PECD) is a recently discovered process with a sensitivity to chirality much larger as compared to traditional (integral) absorption based techniques. Measurements of the chiral asymmetry parameter are performed by detecting the emitted electrons in (and / or in opposite) propagation direction of circularly polarized light, for left versus right polarization.

PTB LABORATORY AT BESSY II

Reconstruction of the spatial distribution of the material composition of periodic nanostructures with grazing incidence X-ray fluorescence analysis

Anna Andrle (Physikalisch-Technische Bundesanstalt, Germany)

Reconstruction of the spatial distribution of the material composition of periodic nanostructures with grazing incidence X-ray fluorescence analysis Poster Abstract (max. 400 characters, no special characters): Si3N4 gratings are analyzed using a method based on GIXRF measurements. The spatial distribution of the material composition of the nanostructures can be reconstructed by calculating the XSW field with a finite element Maxwell solver. A Bayesian optimizer is used to obtain an efficient sampling of the parameter space and to determine the uncertainties of the reconstructed parameters.

Tip-enhanced infrared spectroscopy for the determination of doping concentrations

Richard Ciesielski (Physikalisch-Technische Bundesanstalt, Germany)

We present a theoretical study about the interaction of a metallic nano-probe with doped substrates under the condition of synchrotron radiation in the infrared. Such nano-probes create highly localized fields, which are used for mapping and investigating physical properties on a nanometer length scale. We aim to determine local doping levels by this method, which are otherwise inaccessible.

Using Debye scattering formula for easy numerical calculation of the form factor of arbitrarily shaped nanoparticles regarding small angle X-ray scattering

Jerome Deumer (Physikalisch-Technische Bundesanstalt, Germany)

SAXS is a method to evaluate size distribution of nanoparticles. To gain this information the form factor needs to be known. For many particles the form factor is not known, or it is difficult to calculate resulting in a much higher computational cost. We have developed a method with which the form factor of arbitrarily shaped point clouds can be calculated using Debye's scattering formula.

Upgrade of the x-ray parallel beam facility XPBF 2.0 for characterization of silicon pore optics

Evelyn Handick (Physikalisch-Technische Bundesanstalt, Germany)

The X-ray parallel beam facility (XPBF 2) used for characterizing silicon pore optics (SPO) for the future X-ray observatory ATHENA has been upgraded within the last years. This includes installing a laser-tracker to accurately measure the 12m distance, equipping the cleantent with a cooling unit to keep the temperature at 20°C, replacing the phosphor screen, and to operate the beamline at 1.0 keV.

Traceable and reliable chemical analysis of aerosols by reference-free X-ray spectrometry

Yves Kayser (Physikalisch-Technische Bundesanstalt, Germany)

Reference-free X-ray spectrometry allows for an independent validation of results obtained by means of Total Reflection X-ray fluorescence (TXRF) instrumentation used for high-throughput investigations of particulate matter (PM) collected on substrates. It is shown that grazing incidence X-ray fluorescence measurement allows assessing limits for PM mass which can reliably be quantified using TXRF.

PTB LABORATORY AT BESSY II

A hybrid approach for dimensional nanometrology in semiconductor nanostructures

Leonhard Lohr (Physikalisch-Technische Bundesanstalt, Germany)

The reconstruction of geometrical parameters of semiconductor nanostructures from GISAXS data is often complicated by multi-modalities. In order to resolve this, additional information from complementary fluorescence measurements in the EUVR is used in a hybrid approach. We present a new measurement setup and first results on semiconductor grating structures.

The Optical Constants of Tantalum in the Spectral Range 8 nm - 22 nm

Saadeh Qais (Physikalisch-Technische Bundesanstalt, Germany)

The reconstruction of tantalum optical constants in the spectral range 8 nm - 22 nm is manifested. Reflectivity data collected from a sputtered tantalum thin film via a synchrotron radiation source is used since the optimization of reflectivity data considering an inverse problem allows the simultaneous reconstruction of the two components of the complex refractive index.

Roughness analysis of lamellar gratings using GIXRF

Zanyar Salami (Physikalisch-Technische Bundesanstalt, Germany)

Shrinking the dimensions of nanostructures challenges the existing metrology methods. GIXRF has been used to probe nanoscale features, allowing a dimensional reconstruction. Here, its applicability for the analysis of imperfections on periodic nanostructures is investigated. For the computation of the fluorescence and to explain the possible roughness effects, a Maxwell solver is used.

Element Sensitive Reconstruction of Nanostructures using Grazing Emission X-Ray Fluorescence (GEXRF)

Dieter Skroblin (Physikalisch-Technische Bundesanstalt, Germany)

When combining grazing emission X-ray fluorescence together with ordered nanostructures, features arise in the otherwise homogeneous fluorescence signal. To investigate this behavior, lamellar gratings were examined at the four-crystal monochromator beamline of the Physikalisch-Technische Bundestanstalt. A finite element solver for Maxwell's equations is used to model the measured signal.

The anisotropy in the optical constants of quartz crystals for soft X-rays

Victor Soltwisch (Physikalisch-Technische Bundesanstalt, Germany)

The refractive index of a y-cut SiO_2 crystal surface is reconstructed from polarization dependent soft X-ray reflectometry measurements in the energy range from 45 eV to 620 eV. The anisotropy in the optical constants reconstructed from these data is also confirmed by ab initio Bethe-Salpeter Equation calculations of the O-K edge.

PTB LABORATORY AT BESSY II

Round Robin activity of Total Reflection X-Ray Fluorescence analysis using well characterized, pre-selected samples

Rainer Unterumsberger (Physikalisch-Technische Bundesanstalt, Germany)

In this work, we present the results of a Round Robin test for TXRF analysis of a standard solution. The goal was to separate the TXRF measurement and internal standard based quantification from the sample preparation. The results of the Round Robin test lie within about 5% deviation of all different sample types, showing the strength of the TXRF method when decoupled from the sample preparation.

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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 2021 is

27. November 2020 [00:01] - 10. December 2020 [23:59]

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 voting period 2021 are

Tobias Bock-Bierbaum	Max-Delbrück-Centrum für Molekulare Medizin, Germany
Wolfram Calvet	Technische Universität Darmstadt, Germany
Heiko Peisert	Eberhard Karls Universität Tübingen, 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 the HZB User Committee
Olaf Schwarzkopf	HZB	Representative of the HZB Scientific Director's Office
Franziska Buchner	HZB	Representative of the 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

Mitgliedschaft / Membership

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

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

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

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

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

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

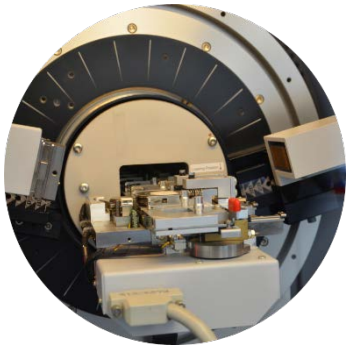
Mitgliedsbeitrag/membership fee: _____ Euro

Im Rahmen freiwilliger Höherstufung/voluntary upgrading: _____ Euro

Datum/date: Unterschrift/signature:

CoreLabs@HZB - Laboratories for International Users and Industry

HZB is setting up CoreLabs a multi-user platform also available for external academic and industrial partners. These CoreLabs are complex infrastructures with unique and state-of-the-art equipment. The main purpose of these CoreLabs is research and development of innovative energy materials.

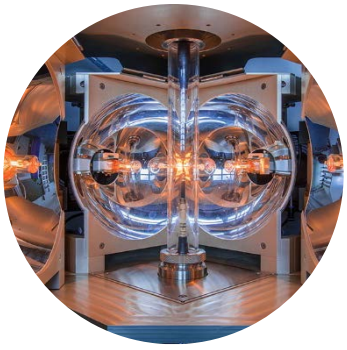


X-ray CoreLab

This CoreLab provides a variety of modern x-ray diffractometers. An outstanding feature of this CoreLab is the in-situ analysis of structural phase transitions, the investigation of structure, microstructure and texture of thin layers, as well as the analysis of internal tensions in materials. The CoreLab also has two MetalJet high-flux x-ray sources providing intense x-ray light with a high brilliance and will open up new perspectives in materials research.

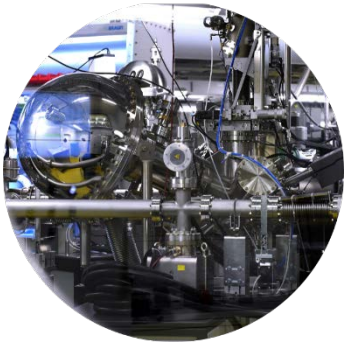
CoreLab CCMS

The CoreLab Correlative Microscopy and Spectroscopy at HZB, is dedicated to support research projects from within HZB by means of electron, ion and light microscopes that are equipped with numerous tools for spectroscopy and materials fabrication. Inquiries from external institutions and companies are welcomed.



CoreLab QM

The CoreLab Quantum Materials offers a suite of instruments and methods for the synthesis and the investigation of new materials relevant for energy and information technologies. The methods are quite general and can be applied to many other material classes. This CoreLab makes them available to all HZB scientists, external scientists in the framework of collaborations, and also commercial users.



EMIL

One part of this multi-user platform is the unique large-scale project EMIL (Energy Materials In-situ Laboratory) located at the synchrotron radiation source BESSY II. EMIL combines soft, tender and hard x-ray spectroscopic methods with a variety of synthesizing, preparation and characterization methods and allows both simultaneous in-situ and operando measurements at several different stations.

Please visit http://hz-b.de/corelabs for more detailed information.

VENDOR EXHIBITION *all-day alongside the meeting*

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MARCH 1, 2021