HZB BESSY II Light Source

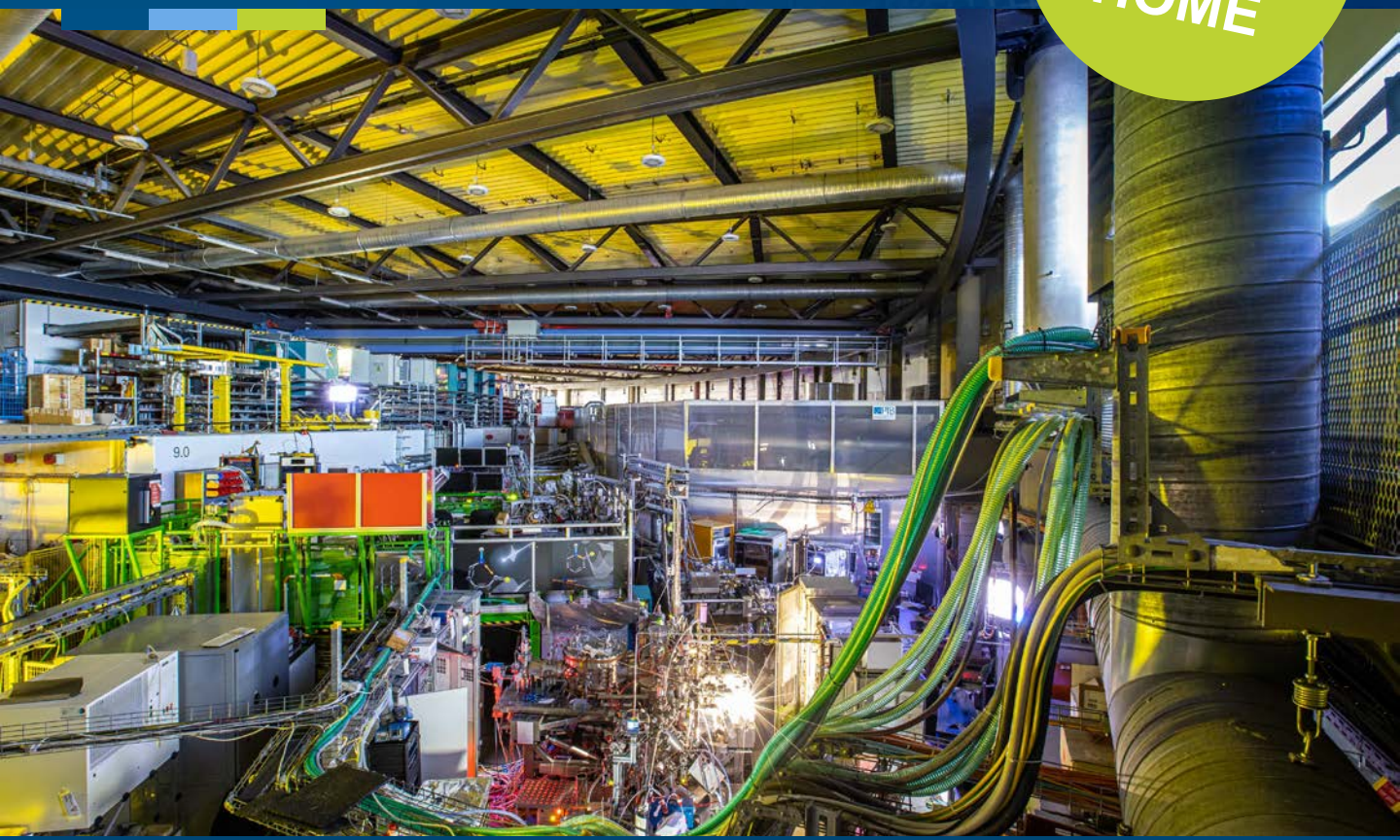
13th BESSY@HZB User Meeting

December 9th, 2021

INVITED SPEAKER

Public Lecture	Robert Schlögl (FHI/MPI CEC)
Life Science & Health	Jan-David Förster (MPIC)
Information Technology	Joachim Gräfe (MPI-IS)
Matter & Material	Sangeeta Sharma (MBI)
Energy Storage	Daniil Itkis (LMSU)
Energy Conversion	Marion Flatken (HZB)

JOIN US FROM HOME



Poster Session Poster Slam Vendor Exhibition

WELCOME

Dear Users and Friends,

Welcome to the 13th BESSY@HZB User Meeting 2021

Looking back over the last year, we have learnt to deal with many unexpected events and to make on-demand adjustments due to the pandemic situation. Unfortunately, for the second time in a row, also our User Meeting is affected and we have to meet in virtual space again.

Nevertheless, we can also look for the silver lining in this situation. Our meeting last year received many encouraging remarks, including those from people who are far away and would not have been able to attend in person. We welcomed participants from Brazil, India and China, the United States and even from Australia. This is an encouraging consolation for all the in-person moments we were not able to enjoy during the online meeting. Almost 500 participants were present online, and we were amazed how much this digital format has reduced the carbon footprint of our User Meeting: More than 80.000 kg CO_2 from at least 300.000 km of travel were saved. Last years' debuts of an awesome poster slam and randomized "carousel" chats were greeted with enthusiasm by the audience and these will be integral parts of our User Meetings to come.

The balancing act between providing the user community with access to the BESSY II facility and taking the necessary measures to protect the health of our employees and users has been the driving force behind further improving the experimental capabilities for remote access at BESSY II, which have been remarkably increased and intensively used by you. Many experiments were performed in a staff assisted manner. During the periods that access to BESSY II was limited to local groups, yet another mode of remote access surfaced: Some of our international users contacted colleagues in Berlin and asked them to do their experiments for them. We would like to thank all of you who helped fulfil our first priority: Maintaining access that is safe for our users.

In 2021, one of the scientific highlights at HZB has been the Kick-Off of the catalysis research laboratory CatLab. HZB and two Max Planck institutes, the Fritz Haber Institute and the Institute for Chemical Energy Conversion, are pooling their expertise and establishing this long-term project together with university and industry partners. The scientific goal is to significantly improve the production process of green hydrogen, which is urgently needed for the energy transition. Towards this goal, CatLab aims at developing novel, tailor-made catalysts using thin-film technologies based on readily available chemical elements and compounds. The research project, which employs unique analytical tools at BESSY II, intends to build a bridge between basic science and industry. We are very grateful to Prof. Dr. Robert Schlögl for presenting CatLab in this year's public lecture.

This year we are also celebrating a special anniversary. The Russian-German Laboratory (RGL) at BESSY II, operating two beamlines and associated experimental stations, is celebrating 20 years of successful operation. In October 2001, the first dipole beamline was completed and since then, the beamlines and stations have continuously been upgraded driven by the evolving needs of the Russian-German user community.

WELCOME

One of the major extensions to the RGL has been the RGBL2 undulator beamline inaugurated in 2019. Congratulations to this long-standing success story and all the best for the years to come!

While these developments are ongoing at BESSY II, we are also busy in preparing its successor, BESSY III. In June, HZB, DESY and HZDR have published a booklet presenting their vision for the long-term development of accelerator-based photon sources in Germany, which perpetuates the successful complementarity of the two German storage ring sources PETRA and BESSY. Thus, BESSY III will focus on spectroscopic and imaging techniques in the soft to tender X-ray range, combining dedicated instrumentation for operando studies with the high brilliance of a 4th generation light source. Also the longstanding and fruitful collaboration with the PTB, enabling metrology with synchrotron radiation, will be continued. Needs of the user community were assessed in a series of expert workshops and are now being incorporated in the compilation of the BESSY III Science Case.

In HZB's research, we have recently taken a leap towards a more sustainable energy supply of our infrastructures: In summer we have commissioned the solar facade of a new building which houses a clean room, various laboratories and assembly stations for HZB's internationally renowned accelerator research. The facade consists of 360 CIGS thin-film solar panels installed on different cardinal directions and serves as a real-world laboratory for photovoltaics research. The panels, which are also an architectural highlight, generate up to 50 kilowatts of electricity and provide important insights into the long-term behaviour of solar modules under different weather conditions.

All research depends on the people doing and enabling it. Therefore, as the first non-university research institution, HZB has successfully completed the audit "Shaping Diversity" (Vielfalt gestalten). The certification attests HZB's efforts to implement concepts and measures that guarantee equal opportunities for diverse groups of people. Regardless of their country of origin, family situation, age, gender, (dis)ability or religion- all employees should be able to participate equally in everyday working life and contribute with their specific abilities. Developing a proper handling of diversity is a key task for scientific workplaces.

Our User Meeting will again underline the broad variety of scientific fields addressed by the experiments realized by you at BESSY II. We will have contributions from outstanding speakers on five major scientific focus areas: energy storage, energy conversion, life science & health, information technology and matter & materials. The Public Lecture on "Sustainable Fuels: BESSY enables conceptual approaches", which Prof. Dr. Robert Schlögl kindly accepted to present, will be another highlight of the programme. Furthermore, we encourage you to contribute with your favourite method of virtual applause for the bestowal of the prizes for Young Scientists' and the European Innovation Award for Synchrotron Radiation.

We will do our best to ensure that, despite its virtual 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 unusual and turbulent times.

Enjoy the meeting!

Sincerely

Prof. Dr. Jan Lüning	Prof. Dr. Bernd Rech
Scientific Director	Scientific Director

CONTENTS

PROGRAMME

13th BESSY@HZB User Meeting on Thursday, 9th of December 2021		
08:00 - 09:00	Registration & Lobby Talk	60 Min.
08:15 - 09:00	Carousel - Match Making Event	45 Min.
09:00 - 10:05	**Synchrotron Session (Chair: Christian Jung)**	**65 Min.**
09:00 - 09:10	Antje Vollmer - Welcome to the User Meeting 2021	10 Min.
09:10 - 09:30	Jan Lüning - 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 - KFS-Chair (KIT) KFS: Synchrotron radiation in Germany and beyond	10 Min
10:00 - 10:05	Cormac McGuinness (ESUO/TCD) An introduction to the European Synchrotron and FEL Users Organisation	05 Min.
10:05 - 10:30	Break: Vendor Exhibition & Lobby Talk	25 Min.
10:30 - 11:30	**Scientific Lectures - Part I (Chair: Annette Pietzsch)**	**60 Min.**
10:30 - 10:50	Life Science & Health - Jan-David Förster (MPIC) Resolving Aerosol Particles and their Atmospheric Processing with X-ray Microspectroscopy	20 Min.
10:50 - 11:10	Information Technology - Joachim Gräfe (MPI-IS) Real-Space Observation of Magnon Interaction with Driven Space-Time Crystals	20 Min.
11:10 - 11:30	Matter & Material - Sangeeta Sharma (MBI) Ultrafast response functions	20 Min.
11:30 - 12:00	Break: Vendor Exhibition & Lobby Talk	30 Min.
12:00 - 12:40	**Scientific Lectures - Part II (Chair: Joachim Breternitz)**	**40 Min.**
12:00 - 12:20	Energy Storage - Daniil Itkis (LMSU)	20 Min.
12:20 - 12:40	Energy Conversion - Marion Flatken (HZB) The Early Stages of Halide Perovskites Thin Film Formation	20 Min.
12:40 - 13:30	Break: Vendor Exhibition	50 Min.
13:00 - 13:30	Carousel - Match Making Event	30 Min.
13:30 - 14:30	**Poster Slam (Chair: Roland Müller)**	**60 Min.**
14:30 - 15:30	**Poster Session - Live chats with poster presenters**	**60 Min.**
15:30 - 16:00	Break: Vendor Exhibition & Lobby Talk	30 Min.
16:00 - 17:00	**Bestowal of Prizes - Friends of Helmholtz-Zentrum Berlin e.V.**	**60 Min.**
17:00 - 17:15	Technical Break	15 Min.
17:15 - 18:15	**Public Lecture - Robert Schlögl (FHI) (Chair: Bernd Rech)** **Sustainable Fuels: BESSY enables conceptual approaches.**	**60 Min.**

ABSTRACTS OF THE SCIENTIFIC LECTURES

SCIENTIFIC TOPICS

Synchrotron User Organisations

Life Science & Health

Information Technology

Matter & Material

Energy Storage

Energy Conversion

Public Lecture

KFS: Synchrotron radiation in Germany and beyond

Jan-Dierk Grunwaldt

KFS-chair, Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

The Committee Research with Synchrotron Radiation (KFS, Komitee “Forschung mit Synchrotronstrahlung", weblink see [1]) is an elected body which represents the interest of more than 4000 synchrotron radiation users (including FELs) in Germany.

Our aim is to act as a link between users and the facilities, between the users and the funding agencies, between Germany and Europe and international sources. In particular, we help to coordinate and to develop strategies for synchrotron radiation applications at national and international sources such as outlined in the recently published strategy paper (“Light for the future” [2]). We want to promote synchrotron research, networking and support especially young enthusiastic researchers and initiatives like NFDI, ErUM-Data and ErUM-Pro (former “BMBF-Verbundforschung“). DAPHNE4NFDI [3] has recently started as a DFG funded project to establish an infrastructure for data storage with data repositories and metadata capture, re-use and joint data analysis software according to the FAIR (findable, accessible, interoperable, reusable) principle.

The KFS is elected every three years, and the last elections took place in autumn 2020. The following scientists were elected/coopted as members for this period:

Jan-Dierk Grunwaldt (chair, Karlsruhe Institute of Technology), Sarah Köster (vice chair, University of Göttingen), Bridget Murphy (University of Kiel), Birgit Kanngießer (Technical University of Berlin), Andrea Thorn (University of Hamburg), Christian Gutt (University of Siegen), Taisia Gorkhover (University of Hamburg), Dirk Lützenkirchen-Hecht (University of Wuppertal), Jochen Geck (TU Dresden), Bernd Hinrichsen (BASF), Manfred Rößle (TH Lübeck) and Max Wilke (University of Potsdam).

In addition, guests representing the German photon facilities BESSY II, DELTA, KIT-Synchrotron, PETRA III, FLASH and the European facilities ESRF and the European XFEL, representatives from funding agencies, PT-DESY and further experts are members.

Do you have topics to be discussed? We are open for opinions, suggestions and questions. Do not hesitate to contact us (Karin Griewatsch, kfsadmin@sni-portal.de).

References and links with further information:

[1] https://www.sni-portal.de/kfs

[2] Strategy brochure: https://www.sni-portal.de/en/news/new-strategy-brochure-of-the-kfs

[3] https://www.daphne4nfdi.de/english

An introduction to the European Synchrotron and FEL Users Organisation (ESUO) & User survey and questionnaire on impact of absence of Trans-National-Access (TNA) funding

Cormac McGuinness[1], Carla Bittencourt[2], Federico Boscherini[2], Tom Hase[2], Rainer Lechner[2], Derek Logan[2], Bridget Murphy[2], Moniek Tromp[2].

1 President of European Synchrotron and FEL Users Organisation ESUO (Trinity College Dublin, Ireland)
2 Executive Board Members of European Synchrotron and FEL Users Organisation ESUO (www.esuo.eu)

The European Synchrotron and FEL Users Organisation (ESUO) was established for the purposes of advocating on behalf of European SR and FEL users of European facilities. ESUO's vision is to support a thriving (European) synchrotron & FEL user community with equal opportunities of access and participation for all scientists based solely on the scientific merit of their ideas.

European users have benefitted over two decades from the availability of financial support via successive Framework/ Horizon 2020 Integrating Activities programmes providing Trans-National-Access (TNA) funding in accessing SR and FEL facilities, paying travel and accommodation costs for one or more members on a beamtime. Earlier in 2014 ESUO had been successfully in helping lobby for the continuation of TNA in Horizon 2020 via general access activity giving the CALIPSOplus programme. TNA was funded by CALIPSOplus until the project ended on 31st October 2021 but with no direct replacement by the European Commission in the form of a general access curiosity driven programme that would continue to provide TNA to all researchers from across Europe no matter the topic.

ESUO has initiated a user survey on the possible impacts of the absence of Trans-National-Access (TNA) funding for the user community. This can be completed by going to the following link: https://www.esuo.eu/possible-impacts-of-the-absence-of-transnational-access-funding-support-for-the-user-community/

All researchers, young and old, whether Master or PhD students, postdoctoral researchers, academic staff, group leaders or professors are encouraged to complete the survey. Using these results, ESUO will continue to advocate to the European Commission, in cooperation with the LEAPS facilities, for TNA funding for all.

ESUO first established in 2010, in 2021 has become an International non-profit organisation, and is composed of national delegates from all European National User Organisations (NUOs) and/or Facility User Organisations (FUOs).

Resolving Aerosol Particles and their Atmospheric Processing with X-ray Microspectroscopy

Jan-David Förster[1], Gholamhossein Bagheri[2], Bruna Holanda[1], Katharina Kaiser[1], Leslie A. Kremper[1], Ovid O. Krüger[1], Mira Pöhlker[1,3], Oliver Schlenczek[2], Johannes Schneider[1], Birte Thiede[2], Markus Weigand[4], Simone Raoux[4], Eberhard Bodenschatz[2], Meinrat O. Andreae[1], Ulrich Pöschl[1], and Christopher Pöhlker[1]

1 Multiphase, Biogeochemistry & Particle Chemistry Departments, Max Planck Institute for Chemistry, Mainz, Germany
2 Laboratory for Fluid Physics, Pattern Formation and Biocomplexity, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany
3 Experimental Aerosol and Cloud Microphysics Department, Leibniz Institute for Tropospheric Research, Leipzig, Germany
4 Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Aerosol particles are ubiquitous in the Earth's atmosphere and impact climate, air quality, and human health on local and global scales. The physico-chemistry of aerosol particles is highly diverse and undergoes significant changes when sojourning the atmosphere from source to deposition. With land-, air-, and sea-based research campaign activities, scientists try to improve our understanding of aerosol-cloud, as well as biosphere-atmosphere interactions. This talk shines spotlights on selected (in-situ) soft x-ray spectromicroscopic investigations conducted at BESSY II and other synchrotrons. The topics covered span from atmospheric aerosols in the Amazon rain forest over polluted urban emissions in east Asia to respiration aerosols in the airborne transmission of pathogens.

References:

J.-D. Förster, I. Bykova, D. S. Macholdt, et al. X-ray Microspectroscopy and Ptychography on Nanoscale Structures in Rock Varnish. *J. Phys. Chem. C.* 125, 22684–22697 (2021).

M. L. Pöhlker, O. O. Krüger, J.-D. Förster, et al., Respiratory aerosols and droplets in the transmission of infectious diseases. *Under review in Reviews of Modern Physics* (2022) (available at http://arxiv.org/abs/2103.01188).

J.-D. Förster, C. Gurk, M. Lamneck, et al. MIMiX: a Multipurpose In situ Microreactor system for X-ray microspectroscopy to mimic atmospheric aerosol processing. *Atmos. Meas. Tech.* 13, 3717–3729 (2020).

Real-Space Observation of Magnon Interaction with Driven Space-Time Crystals

Nick Träger[1], Paweł Gruszecki[2], Filip Lisiecki[3], Johannes Förster[1], Felix Groß[1], Markus Weigand[1,5], Piotr Kuświk[3,4], Janusz Dubowik[3], Gisela Schütz[1], Maciej Krawczyk[2], Joachim Gräfe[1]

1 Max Planck Institute for Intelligent Systems, Stuttgart, Germany
2 Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
3 Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
4 Centre for Advanced Technology, Adam Mickiewicz University, Poznań, Poland
5 Helmholz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

In analogy to conventional space crystals in condensed matter and atomic physics, Wilczek proposed the theory of spontaneous breaking of time symmetry and the emergence of Time Crystals [1]. Furthermore, a simultaneous crystalline formation in space permits the emergence of discrete space-time crystals (STC). Experiments confirmed the existence in abstract quantum systems [2].

Here, we directly observe lattice scattering on a driven STC within a magnonic Py waveguide [3]. Due to the generated periodicity in space and time, a band structure is formed and mode folding at the first Brillouin has to be taken into account. Therefore, magnons can scatter at the driven STC into higher spatial frequencies, which are forbidden in the conventional dispersion relation theory for the same structure (cf. Fig. 2).

These scattering processes are observed and imaged in real space by scanning transmission x-ray microscopy (STXM) with magnetic contrast that features the necessary spatial (< 20 nm) and temporal (< 40 ps) resolution. The initial formation of the driven STC is caused by a continuous wave (CW) global radio frequency field, which leads to spin wave emission from the left and right edge of the waveguide [4]. Consequently, a standing spin wave pattern arises revealing oscillation in space and time (cf. Fig. 1).

With the realization of a driven space-time crystal in magnonic waveguides, we take the abstract idea of space-time crystalline structures to the next level and reveal new phenomena in the field of non-linear wave physics. These fundamental findings could pave the way for reconfigurable magnonic crystals without nanoscale patterning and for a new generation of spin wave emitter at ultra short length scales.

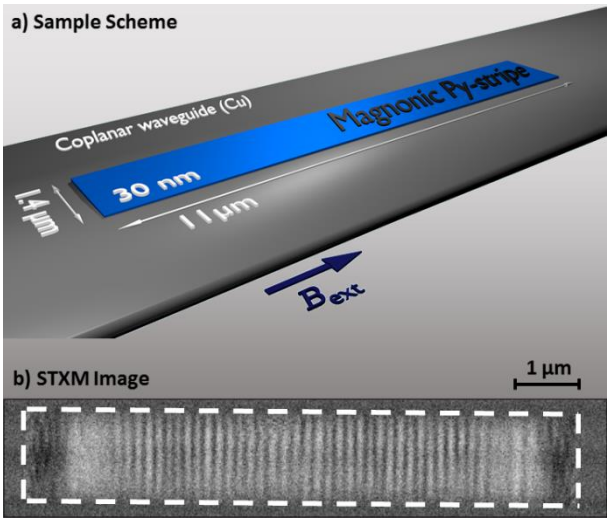


Fig. 1: (a) Sketch of the Magnonic Py waveguide (blue) with the coplanar waveguide (gray). (b) STXM image during continuous wave RF excitation. The grayscale represents the m_z component.

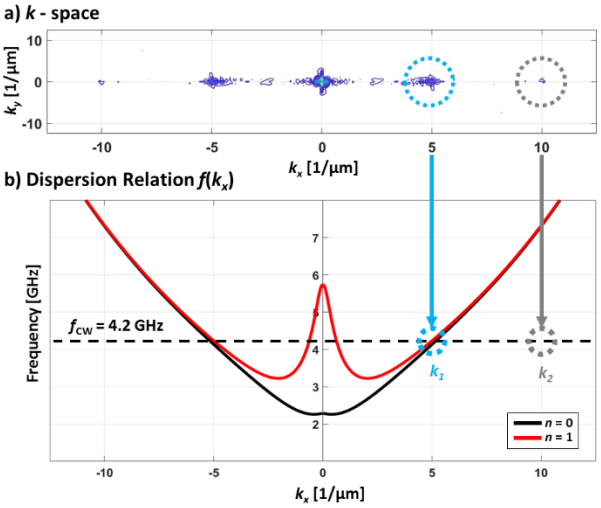


Fig. 2: (a) k-space image of the excited standing spin wave pattern. (b) The dispersion relation $f(k_x)$ shows the CW excitation f_{CW}. The mode numbers n = 0 and n = 1 are depicted in black and red, respectively. Folding of bands due the formation of a space-time crystalline structure explains the double spatial frequency of k_2.

References:

[1] Wilczek, F., Quantum Time Crystals. PRL, 2012. 109(16): p. 160401.

[2] Smits, J. et al., Observation of a Space-Time Crystal in a Superfluid Quantum Gas. PRL, 2018. 121(18): p. 185301.

[3] Träger, N. et al., Real-Space Observation of Magnon Interaction with Driven Space-Time Crystals PRL, 2021. 126(5): p. 057201.

[4] Mushenok, F. B. et al., Broadband conversion of microwaves into propagating spin waves in patterned magnetic structures. APL, 2017. 111(4): p. 042404.

Ultrafast response functions

Sangeeta Sharma

Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Straße 2A, 12489 Berlin

Ultrafast magnetization dynamics induced by femtosecond laser pulses is a rapidly developing research field. This is due to the vast increase in speed that such processes offer over traditional methods of magnetic manipulation. Due to short timescales and the push towards smaller length scales, the problem is intrinsically quantum-mechanical and thus challenging to understand and predict. In this regard, both theory and experiment must work together in order to comprehensively understand the problem. However, it has been difficult for theory and experiments of work in tandem in the field due to the fact that the experimental observables are often indirect measurements of those that are simulated; experiments rely on spectroscopy to study transient magnetization dynamics. In theoretical work on femtomagnetism on the other hand, the fundamental quantity calculated is the dynamics of the spin magnetic moment itself [1-4,7,8,9].

The ability to measure and calculate the same physical quantity thus forms the cornerstone of the vital collaboration between theory and experiment, and I will discuss recent work where we have *ab-initio* calculated the real time response functions of L-edge and M-edge semi-core states during spin dynamics, demonstrating both good quantitative agreement with experiment [5,6] but also showing how theory can actually predict new phenomena and guide new experiments.

References:

[1] Dewhurst et al. Nano Lett. 18, 1842, (2018)

[2] Elliott et al. Scientific Reports 6, 38911 (2016)

[3] Shokeen et al. Phys. Rev. Lett. 119, 107203 (2017)

[4] Chen et al. Phys. Rev. Lett. 122, 067202 (2019)

[5] Willems et al. Nat. Comm. 11, 1 (2020)

[6] Dewhurst et al. Phys. Rev. Lett. 124, 077203 (2020)

[7] Hofherr et al. Sci. Advs. 6, 8717 (2020)

[8] Siegrist et al. Nature 571, 240 (2019)

[9] Golias et al. Phys. Rev. Lett. 126, 107202 (2021)

ENERGY STORAGE *12:00 - 12:20*

The Early Stages of Halide Perovskites Thin Film Formation

Marion A. Flatken

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

The solution-based fabrication procedure of perovskite solar cells is one criterion that makes them particularly well suited for rapid and cost-efficient manufacturing with respect to future commercialization. The relationship between solution properties, crystal quality and final solar cell performance serves as motivation for the presented project, highlighting the importance of fundamental insights about the precursor chemistry of metal halide perovskites towards polycrystalline thin film formation. The combination of spectroscopic and synchrotron based scattering characterization techniques provides a comprehensive picture of their complex colloidal chemistry. In this sense, we elaborate relevant parameters to influence systematically the perovskite crystallization for morphology control, paving the way towards commercial application of tailor made perovskite solar cells.

Hence, in this study we provide a comprehensive picture of the complex precursor chemistry of metal halide perovskites. We introduce comprehensive insights covering a broad range of parameters, such as (I) the external implications based on concentration and temperature (II) the addition of counter ions to reduce the diffuse layer surrounding the NPs and (III) the targeted use of additives to eliminate selectively unwanted components to ensure a more homogeneous crystal growth.

PUBLIC LECTURE *17:15 - 18:15*

Sustainable Fuels: BESSY enables conceptual approaches

Robert Schlögl

1 Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin
2 Max-Planck-Institute for Chemical Energy Conversion, Stiftstr. 34-36, 45470 Mülheim an der Ruhr

The energy challenge will require to a massive extent the use of sustainable generated molecules as energy carriers. Hydrogen is the primary platform molecule. It can come from water splitting but also for dehydrogenation reaction of fossil and biological hydrocarbons as long as no CO2 is co-generated.

But hydrogen is not the best energy carrier when considered for long-distance transport and for distributed end use. This derivatives of hydrogen such as ammonia, LOHC and alcohols generated from unavoidable CO2 and hydrogen will play an important role in future energy systems.

The conversion of free electrons in molecules and its further derivatisation is unthinkable without catalysis. Interfacial catalysis will play the dominant role. As well as we understand today the interface between a solid and its surrounding reactants, as poor is our understanding about the other functional interfaces in the system. Here the project CatLab will make a strategic contribution. Based on the dynamic action of the heterogeneous interface it is of utmost importance to prevent undesired surface phase changes during operation that de-activate the working catalyst. This is controlled through the buried interfaces present in the system. These are the targets to be studied and modified synthetically within the Catlab project. The presentation will indicate the underlying science concept and illustrate how Catlab works as cooperation project between HZB and MPG supported by additional partners.

PLEASE NOTE

The Public Lecture will be streamed live on

https://zoom.us/j/92634833019?pwd=VWo4SHdmMWw0aC9Gc1E2bzN4QWVQZz09

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

POSTER SLAM - PARTICIPANTS *13:30 - 14:30*

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 PTB Laboratory at BESSY II / Life Science & Health

Quantitative and qualitative characterisation of trace elements in pancreatic and pancreatic carcinoma sections of mice by reference-free X-ray fluorescence analysis

Katja Frenzel (Physikalisch-Technische Bundesanstalt, Germany)

2 UE46_MAXYMUS / Matter & Material

History dependent skyrmion and domain formation in van der Waals magnet Fe_3GeTe_2

Max Birch (Max Plank Insitute for Intelligent Systems, Germany)

3 U41-TXM / Matter & Material

Study of metal-carboxylate complex derived from Pinus elliotti resin applied as antibacterial and antifungal pigment in home paints

Carla Bittencourt (University of Mons, Belgium)

4 U49-2_PGM-1 / Matter & Material

Expanding Liquid-Jet Photoelectron Spectroscopy to Free-Flowing Planar Surfaces

Dominik Stemer (Fritz-Haber-Institut, Germany)

5 Information Technology

FAIR and open data for national photon and neutron facilities in Europe

Sophie Servan (Deutsches Elektronen-Synchrotron, Germany)

6 UE48_EMIL / Matter & Material

Unravelling the Effect of superficial Rh depletion on shallow d-states of Gallium-Rhodium Liquid Metal Alloys

Tzung-En Hsieh (Helmholtz-Zentrum Berlin, Germany)

7 UE49_PGM SMART / Matter & Material

The relation of structure sensitivity and doping of ceria [(111) vs (100)] for CO_2 hydrogenation

Emilia Pozarowska (BTU Cottbus-Senftenberg)

8 HE-SGM

Spectroscopic studies of on-surface synthesis of chiral graphene nanoribbons on Au(788)

Igor Chunin (Trinity College Dublin, Ireland)

9 MX Beamline / Life Science & Health

Hundreds of starting points to develop protein-protein interaction modulators

Tatjana Barthel (Helmholtz-Zentrum Berlin, Germany)

POSTER SLAM

10 *KMC-1 / Matter & Material*

Induced reduction by H2 exposure at room temperature of ceria ultrathin films grown by atomic layer deposition

Carlos Morales (BTU Cottbus-Senftenberg, Germany)

11 *UE52_PGM Nano cluster trap / Matter & Material*

XAS study of electronic structure and oxidation states of manganese atoms in cold gas-phase $Mn_2O_x(H_2O)^{n+}$ clusters.

Olesya Ablyasova (Helmholtz-Zentrum Berlin, Germany)

12 *Life Science & Health*

Decoding how cell fate reprogramming transcription factors activate epigenetically silenced chromatin

Daisylyn Senna Tan (The University of Hong Kong)

13 *BAMline / Information Technology*

X-ray prism illumination optics

Arndt Last (Karlsruhe Institute of Technology, Germany)

14 *KMC-1 / Energy Conversion*

Impact of the IZO sputter deposition on the underlying C60/metal halide perovskite top cell interface as revealed by direct and inverse photoemission

Elif Hüsam (Helmholtz-Zentrum Berlin, Germany)

15 *UE46_MAXYMUS / Matter & Material*

Demonstrating optical-pump-x-ray probe experiments at 50 MHz repetition rate on a solid-state sample

Kathinka Gerlinger (Max-Born-Institute, Germany)

16 *Other Topic*

LEAPS IDEA – Inclusion, Diversity, Equity, and Anti-discrimination

Antje Vollmer (Helmholtz-Zentrum Berlin, Germany)

17 *BAMline / Energy Storage*

3D visualization of the phase transformation of µm-CuS in SSBs

Zhenggang Zhang (Humboldt Universität zu Berlin, Germany)

18 *PTB Laboratory at BESSY II / Matter & Material*

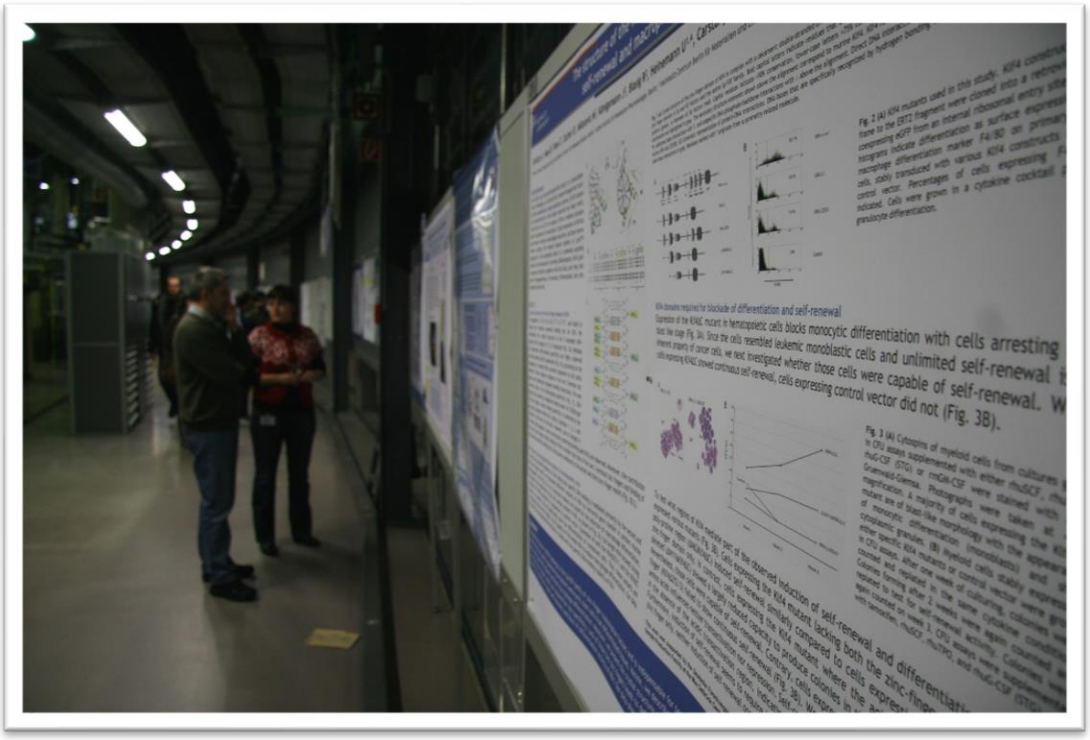
Investigation of halide perovskite precursor solutions with small-angle X-ray scattering (SAXS)

Ana Palacios Saura (Helmholtz-Zentrum Berlin, Germany)

19 *MX Beamline / Life Science & Health*

Fragment based design of mycobacterial thioredoxin reductase inhibitors: from a fragment screening to novel inhibitors.

Friederike Theresa Füsser **(**Westfälische Wilhelms-Universität Münster, Germany)



SCIENTIFIC TOPICS

Energy Conversion

Energy Storage

Information Technology

Life Science & Health

Matter & Material

Other

PTB Laboratory at BESSY II

Pd Thin Film Catalysts

Eylül Öztuna (Helmholtz-Zentrum Berlin, Germany) *BElChem-PGM*

We have studied thin films of Palladium deposited on Si, SiO_2 and ZnO for catalytic application in selective acetylene hydrogenation by means of X-ray spectroscopy, electron microscopy, and theoretical simulation to elucidate stability issues of the film and try to understand the relationship to their activity and selectivity.

Temperature-dependent FTIR-studies of composite proton conducting membranes with nanodiamonds

Yuri Kulvelis (Petersburg Nuclear Physics Institute, Russia) *IRIS*

Perfluorinated membranes have great prospects for the use in hydrogen fuel cells. Nanodiamonds embedded in the polymer matrix provide an increase in proton conductivity, depending on the nanodiamond type and content. The presence of nanodiamonds makes changes in FTIR-spectra in hydration/dehydration process (smoothing of the local peaks, responsible for interaction with water molecules).

Design and Fabrication of Solid Oxide Model Cells for Synchrotron-based Operando Studies

Mauricio Arce (Helmholtz-Zentrum Berlin, Germany) *ISISS*

Synchrotron-based operando techniques are a key for studying solid oxide cells. In this work we focus on the design, fabrication, and characterization of a model cell for operando studies, showing some selected examples where they are employed. These cells consist of a $Sr(Ti,Fe,Ni)O_3$ thin film electrode deposited by PLD on YSZ single-crystal electrolyte and a highly active Pt counter-electrode.

Formation of oxygen vacancies during high OER potentials

Steffen Czioska (Karlsruhe Institute of Technology, Germany) *ISISS*

Electrochemical oxygen evolution reaction (OER) catalysts are mainly investigated at low potentials. Recently, we investigated IrO_2 at high OER overpotentials by different in-situ X-ray absorption techniques. A change in mechanism was observed compared to lower voltages, caused by the formation of oxygen vacancies. These results were further confirmed by in-situ XPS measurements at ISSIS beamline.

Tuning the surface exsolution of Ni-Fe nanoparticles from Ni-doped $Sr(Ti,Fe)O_{3-\delta}$ thin-film electrodes for symmetric SOFC/SOEC devices: Insight from operando ambient pressure-XPS and -NEXAFS studies

Catalina Jimenez (Helmholtz-Zentrum Berlin, Germany) *ISISS*

Solid oxide fuel and electrolyzer cells (SOFC and SOEC) are considered key for a sustainable energy system. Ni-doped $Sr(Ti,Fe)O_{3-d}$ exsolves Ni-Fe nanoparticles that enhance the H_2 oxidation reaction (HOR) by catalyzing the H_2 adsorption. Our operando study reveals how electrode polarization affects exsolution in relation to temperature and chemical potential of the atmosphere in SOFC/SOEC cycles.

Impact of the IZO sputter deposition on the underlying C60/metal halide perovskite top cell interface as revealed by direct and inverse photoemission

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

Wide-bandgap metal halide perovskites (HaP) can form top-cells in tandem photovoltaic devices, which contain several layers and interfaces which crucially influence the power conversion efficiency (PCE). We present analysis of the C60/HaP stack – focusing on changes induced by rf-sputter deposition of IZO – using ultraviolet (UPS), x-ray (XPS), and inverse (IPES) photoelectron spectroscopy.

HAXPES & XAS measurements on BA_2PbI_4 2D-crystals: Challenges and potential mitigation strategies

Ahmed Saleh (Helmholtz-Zentrum Berlin, Germany) *KMC-1*

2D halide perovskites, HaPs, are more ambient-stable than analogous 3D ones. We performed first HAXPES and XAS measurements on single crystals of (butyl-ammonium)$_2PbI_4$, a 2D HaP, at HiKE/KMC-1. We found and report here on serious challenges that such experiments face, specifically sample degradation and charging. Possible strategies to mitigate, bypass or overcome these problems will be presented.

Evaluating NP Exsolution, Reabsorption, and Degradation Mechanisms of Ni-doped $Sr(Ti,Fe)O_3$ Thin-film Electrodes by Operando Grazing Incidence X-Ray Diffraction

Mauricio Arce (Helmholtz-Zentrum Berlin, Germany) *KMC-2*

Electrocatalytically active nanoparticle (NP) exsolution and reabsorption on SOFC electrodes can be triggered by treatment atmosphere and electrode polarization. We have studied these processes by operando GIXRD on Ni-doped $Sr(Ti,Fe)O_3$ thin-film electrodes, while detecting secondary phases produced on the surface and electrode-electrolyte interface, that can lead to degradation of FC performance.

Group-Subgroup Relationships in Wurtzite-related Nitrides

Joachim Breternitz (Helmholtz-Zentrum Berlin, Germany) *KMC-2*

A vast number of materials crystallise in the wurtzite-type or one of its subgroups. The different cation orderings and structural distortions in this class of materials open a rich variety of different crystal structures in subgroups of the wurtzite-type. We establish a structural-systematic of this class for nitride materials, which culminates in the establishment of a Bärnighausen tree.

In-situ characterization of ZrO_2 and YSZ thin films for energy applications

Yanet Mansilla (Centro Atómico Bariloche, Argentina) *KMC-2*

Properties of zirconia-based thin films are highly depend on the crystallite size, thus on the synthesis conditions. We study in-situ the crystallization process of ZrO_2 and YSZ films by GIXRD and their electrical properties by measurements of electrical conductivity. These results allow to follow the evolution of the crystal structure with the temperature and to optimize the synthesis.

ENERGY CONVERSION *BEAMLINE*

MEAD and cation order in kesterite-type semiconductors

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

Cation order in multiple quaternary chalcogenide semiconductors of kesterite- and wurtz-kesterite structure has been determined using Multiple Edge Anomalous Diffraction. MEAD allows to lift correlation problems of structural parameters and provides results in a particularly convincing way.

High-Throughput Analysis of Combinatorial Lead Halide Perovskite Libraries through GIWAXS Mapping

Hampus Näsström (Helmholtz-zentrum Berlin, Germany) ***mySpot Beamline***

For high-throughput materials discovery we characterize combinatorial libraries of $CsPb(Br_xI_{1-x})_3$, manufactured in the HySPRINT laboratory, with in-situ grazing incidence wide angle X-ray scattering, GIWAXS, at the mySpot BESSY beamline and the metaljet source of the X-ray CoreLab. We determine the temperature dependent phase diagram of $CsPb(Br_xI_{1-x})_3$ and the local spatial compositional homogeneity.

Interface investigation of thickness gradients of Ir and IrOx thin films on TiO_2 for OER catalyst applications by x-ray spectroscopies

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

Thickness-gradient thin film libraries of Ir/TiO_2 and IrO_x/TiO_2 were prepared using magnetron sputtering to investigate the chemical interface structure by means of soft and hard XPS and Ti L2,3- and O K-edge XAS. This study explores the influence of the interface properties on the OER activity and stability as a function of both annealing temperature and iridium (oxide) layer thickness.

Chemical and Electronic Structure Profiles of Silver-Alloyed $Cu(In,Ga)Se_2$ Thin-Film Solar Cell Absorbers

Donald Valenta (Helmholtz-Zentrum Berlin, Germany) ***UE48_EMIL***

Silver-alloying of $Cu(In,Ga)Se_2$ chalcopyrites can reduce structural defects, improve their opto-electronic properties, and thus potentially enhance the performance of respective solar cell devices. Fully exploiting the exceptionally wide photon energy range of EMIL's two-color beamline, we studied the chemical and electronic structure profiles of $(Ag,Cu)(In,Ga)Se_2$ thin-film solar cell absorbers.

Investigation of the Oxidation Mechanism of H_3PO_3 on Pt Through X-ray Spectroscopies

Enggar Wibowo (Helmholtz-Zentrum Berlin, Germany) ***UE48_EMIL***

Several studies indicate the generation of phosphorus acid (H_3PO_3) during operation of high-temperature polymer electrolyte membrane fuel cells using phosphoric acid (H_3PO_4) as electrolyte. This study aims at elucidating the interaction of H_3PO_3 with the Pt electrode ultimately revealing its oxidation mechanism back to H_3PO_4, through in-situ P K-edge XAS and complementary ex-situ XPS measurements

Transient NEXAFS measurements of organic thin films with synchrotron and laboratory sources

Richard Gnewkow (Helmholtz-Zentrum Berlin, Germany) ***UE56-1_PGM***

Transient NEXAFS measurements on thin films can be done at synchrotron and laser-based laboratory sources. Measuring thin films in the pump-probe scheme is however demanding due to radiation damage. Additionally, sample heating influences the measured spectra. Differences between synchrotron and laboratory pump-probe measurements of organic thin films and ways to minimize radiation damage will be presented.

Nitrogen/Carbon-Coated Zero-Valent Copper as Highly Efficient Co-catalysts for TiO_2 Applied in Photocatalytic and Photoelectrocatalytic Hydrogen Production

Lucy Ombaka (Technical University of Kenya)

The in-situ encapsulation of Cu nanoparticles inside N-graphitic carbon layers (14.4 % N) is utilized to stabilize Cu nanoparticles (N/C-coated Cu) and improve its electronic communication with a TiO_2 photocatalyst. N/C-coated Cu/TiO_2 composites outperforms its uncoated Cu counterparts, achieving an excellent rate H_2 evolution rate of 19.03 mmol $g^{-1}h^{-1}$.

CatLab@EMIL: Tailored thin film deposition for catalysis research at BESSY II

Alexander Steigert (Helmholtz-Zentrum Berlin, Germany)

The aim of the CatLab project is to explore a novel concept for the production of high-performance catalysts. SISSY@EMIL with deposition and analytics in one system offers optimal conditions. First systems currently being investigated are based on ultra-thin Pd films deposited on homogeneous support materials; with the latter impacting interface structure and catalytic performance.

3D visualization of the phase transformation of µm-CuS in SSBs

Zhenggang Zhang (Humboldt Universität zu Berlin, Germany) ***BAMline***

Understanding the bulk structural evolution of materials during electrochemical reactions and its effect on solid-state batteries (SSBs) is critical, but has been rarely studied due to problems with traditional technologies being able to detect bulk information in SSBs. In this study, CuS was taken as a model material for its high capacity, high conductivity, and large volume variation.

How to benefially restructure an OER catalyst?

Javier Villalobos (Helmholtz-Zentrum Berlin, Germany) ***KMC-3***

Erythrite mineral was used as a study model to evaluate the catalytic properties during electrochemical restructure into a Co-based oxide in four different electrolytes. Only carbonate can activate the catalytic material, attributed to: an adequate local order, a high Co oxidation state and high number of redox-active Co ions. These requirements provide new insights into the design of OER catalysts.

How PEAXIS helps unravel the mystery of O-redox cathodes for Li-ion batteries through Resonant Inelastic X-ray Spectroscopy

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

Next generation cathodes of Li-ion batteries have utilized the presence of an additional redox reaction that added extra capacity to store charge. At PEAXIS, soft X-ray resonant inelastic spectroscopy (RIXS) measurements were used to probe the associated oxygen product that is formed. The results help develop and tailor materials that can further improve their battery capacity performance.

Surface chemistry of 2,3-dicyanosubstituted norbornadiene/quadricyclane on Ni(111)

Felix Hemauer (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany) ***UE56-2_PGM-2***

The results of 2,3-dicyanosubtitued norbornadiene/quadricyclane on Ni(111) as model system for heterogeneously catalyzed energy release are discussed. With a reasonable size and a red-shifted absorption onset of at least 40 nm in comparison to parent NDB, the adsorption and thermal evolution of (CN)2 NBD and (CN)2-QC was investigated.

X-ray prism illumination optics

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

X-ray prism lenses (XPL) with prism edge lengths of 20 µm and physical apertures of up to 1.8 mm x 1.8 mm are developed at KIT/IMT and manufactured by X-ray deep lithography at the KIT Synchrotron radiation source. They serve as highly transparent illumination optics for sample illumination and in full-field X-ray microscopy. We present results of the optical characterisation of such XPLs.

Ultra-short helix pitch and spiral ordering in cholesteric liquid crystal revealed by resonant soft X-ray scattering

Alevtina Smekhova (Helmholtz-Zentrum Berlin, Germany) ***UE52_SGM***

A newly synthesized liquid crystal material with a single lactate unit in a molecular chain reveals the shortest up-to-now reported value of the helix pitch in the cholesteric phase at room temperature. The pitch of 104 +/- 1 nm and the size of coherently scattering domains (approx. 500 nm) were directly probed by the resonant soft X-ray scattering (RSoXS) near the carbon K-edge resonance.

HMC Hub Matter@HZB

Oonagh Mannix (Helmholtz-Zentrum Berlin, Germany)

Survey, use case, training, electron microscopy…. Come and find out what Hub Matter of the Helmholtz Metadata Collaboration has been doing for the past year. Learn how to get involved with our activities for the next year. We can also answer questions about what is happening in the world of metadata in the Helmholtz Association, Germany, Europe and beyond.

FAIR and open data for national photon and neutron facilities in Europe

Sophie Servan (Deutsches Elektronen-Synchrotron, Germany)

To make photon and neutron data FAIR, the H2020 ExPaNDS project provides a framework for EU PaN facilities to work together to produce data that can be easily shared and re-used. Our work on metadata, persistent identifiers, standardised interfaces to data catalogues and portable analysis workflows make for better reproducibility and interoperability in science, across borders and disciplines.

X-ray refraction radiography applied to Dental Fibre Posts

Frank Wieder (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

Fibre-Matrix-Debonding in glass fibre reinforced dental posts can play an important role for their mechanical performance and long term stability… We show that synchrotron X-ray refraction radiography (SXRR) allows analysis of large samples (up to several millimetres) without compromising the detectability of sub micrometer defects.

Wrapping and blocking of Influenza A Viruses by Sialylated 2D Nanoplatforms

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

Inhibition of respiratory viruses is one of the most urgent topics as underlined by different pandemics in the last decades. This impels the development of new materials for binding and incapacitation of the viruses. In this work, we demonstrated that an optimal deployment of influenza A virus targeting ligand sialic acid on a flexible 2D platform enables its binding and wrapping around virus particles.

Exploring the interplay between microplastics and biofilms in freshwater

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

Plastic inevitably accumulates in the environment becoming a persistent. In the present work, we aim at documenting MPs occurrence in three collection spots of the biggest European artificial lake over one year period using infrared microscopy. Scanning electron microscopy was used to evaluate MPs colonization by biofilms. PE was the most abundant polymer and biofilms were identified in all plastics.

Tryptophan regulates Drosophila zinc stores

Nils Schuth (Centro de Investigación y de Estudios Avanzados, Mexico) ***KMC-3***

Zinc deficiency is commonly attributed to inadequate absorption of the metal. Instead, here we show in vivo that body Zn stores in Drosophila melanogaster depend on tryptophan consumption. Hence, a dietary amino acid regulates Zn status of the whole insect – a finding consistent with the widespread requirement of Zn as a protein cofactor.

Hundreds of starting points to develop protein-protein interaction modulators

Tatjana Barthel (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.

Fragment based design of mycobacterial thioredoxin reductase inhibitors: from a fragment screening to novel inhibitors.

Friederike Theresa Füsser (Westfälische Wilhelms-Universität Münster, Germany) *MX Beamline*

For the identification of new starting points for the development of antituberculotic drugs, a crystallographic fragment screening was performed. The diffraction data were collected at BESSY II and analysed by the automated software pipelines at HZB including hit identification via PanDDA. 40 fragments and four promising binding sites were found and will be used for further investigations.

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

Thomas Hauß (Helmholtz-Zentrum Berlin, Germany) *MX Beamline*

XDSAPP3 is a further development of the well-known program XDSAPP [Sparta, K. et al. (2016). J. Appl. Cryst. 49] to (semi-) automatically process diffraction data using XDS [Kabsch, W (2010) Acta Cryst. D66]. Improvements in decision making, the support for EIGER detectors, and additions to the GUI are some of the major advances. XDSAPP3 will run on recent Linux and MacOS operating systems.

TBEV RNA-Dependent RNA Polymerase - Structure and Interactions

Petra Havlickova (University of South Bohemia, Czech Republic) *MX Beamline*

RdRp is an essential protein for TBEV RNA replication. It plays a significant role in the membrane-associated replication complex where it interacts with NS3 helicase. This project is focused on the structure determination of RdRp as well as on its interactions with RNA and NS3 helicase, using methods such as X-ray crystallography, cryo-EM, fluorescence polarization, HDX etc.

Visible-Light Removable Photocaging Groups Accepted by MjMAT Variant

Eric Herrmann (Westfälische Wilhelms-Universität Münster, Germany) *MX Beamline*

Methylation of biomolecules is a major regulatory mechanism involved in epigenetic and epitranscriptomic processes. Investigations would benefit from the ability to install photo-cleavable groups, removable by non-damaging light, at methyltransferase target sites. Therefore, we characterized MjMAT variations in complex with S-Adenosyl-L-methionine (AdoONB) and red-shifted derivative thereof.

Ixodes ricinus serpins

Barbora Kascakova (University of South Bohemia, Czech Republic) *MX Beamline*

I. ricinus, hard ticks, have a wide geographical distribution mainly in Europe. Tick is a long-time bloodsucking parasite in all developmental stages that modulate host defense mechanism due to the feeding process that takes several days until repletion. For this, tick saliva contains antihemostatic and immunomodulatory molecules mainly serpins that irreversibly inhibit their targets.

Fragment screening workflow for MX users at BESSY II

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

At the macromolecular crystallography (MX) beamlines at HZB, a user workflow provides for efficient fragment screening. It includes dedicated tools, the diverse F2X compound libraries and largely automated software pipelines. Identified binders present starting points for tool compound development or drug discovery. Subsequent fragment evolution towards higher potency is possible via Frag4Lead.

Investigating the cellular mechanism of coronavirus inhibition by anti-depressants

James McNally (Helmholtz-Zentrum Berlin, Germany) ***U41-TXM***

FDA-approved anti-depressant drugs have been shown to inhibit coronavirus replication in cell culture models and also to reduce hospitalization in high-risk patients, but their mechanism of action remains unknown. Combining X-ray, fluorescence and electron microscopy, we find these drugs may inhibit either uptake of the virus by filopodia or release of the virus from late endosomes.

Microstructure and chemistry of expiratory aerosols in the airborne transmission of pathogens

Jan-David Förster (Max-Planck-Institut für Chemie, Germany) ***UE46_MAXYMUS***

With soft x-ray spectromicroscopy, we characterized the morphology, phase state, and chemical composition of respiratory particles emitted upon breathing, singing, shouting, etc. and found distinct patterns. As airborne pathogen-laden particles, these properties largely affect their residence time in air, long-range transmission, lung deposition, and thus health effects.

Site-selective soft X-ray absorption as a tool to study protonation and electronic structure of gas-phase DNA

Thomas Schlathölter (University of Groningen, Netherlands) ***UE52_PGM Nano cluster trap***

Conformation and electronic structure of gas-phase DNA depends strongly on the protonation site. We used the IonTrap setup for soft X-ray spectroscopy on protonated 5'-d(FUAG). N K-edge spectra were compared to time-dependent density functional theory calculations using a short-range exchange correlation functional. Best agreement between experiment and theory was found for A-N1 protonated oligonucleotides.

Investigating the Structural Dynamics of the Water and Proton Channels Using snap-shots of Photosystem II

Rana Hussein (Humboldt Universität zu Berlin, Germany)

The water oxidation process in Photosystem II, a Bio-machinery that evolved nearly three billion years ago, fascinates us with its capabilities of harvesting solar energy and storing it in a chemical form. The X-ray Free Electron Lasers enabled us to study this phenomenal protein in ways that were not possible before. In the current study, we employed SFX and XES at room temperature (RT) to investigate PSII.

Decoding how cell fate reprogramming transcription factors activate epigenetically silenced chromatin

Daisylyn Senna Tan (The University of Hong Kong)

Pioneer transcription factors (PTFs) have an ability to bind silenced DNA that is methylated or compacted in chromatin. Pioneer factors are often involved in cell fate reprogramming used in regenerative medicine. However, biochemical evidence of how these TFs directly binds silenced DNA is sparse. Here, we study the binding of OCT4,a key PTF, and BRN2 towards methylated DNA and nucleosome core particles.

Metal-doped ZnO nanopowder via Green Chemistry: dopant location and local structure to understand antibacterial activity

Carla Bittencourt (University of Mons, Belgium) ***BAMline***

ZnO nanoparticles obtained by green synthesis using Cassava Starch a biocompatible polysaccharide, are paint pigment. Metal doping extend their applications as pigments with antibacterial activity. Using XAFS at the K-edges of 3d-transition metals and L3-edges of rare earth metals we explore the chemical state and the local coordination of metal dopants and correlate with antibacterial activities.

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 even within seconds.

Synchrotron X-Ray Refraction during in-situ heat treatments

Itziar Serrano-Munoz (Bundesanstalt für Materialforschung und -prüfung, Germany) ***BAMline***

For the first time, synchrotron X-ray refraction radiography (SXRR) has been paired with in-situ heat treatment to monitor microstructure and porosity evolution as a function of temperature.

Magnetron sputter deposition of copper onto liquids: understanding the chemical post synthetic transformations of copper nanoparticles

Anastasiya Sergievskaya (University of Mons, Belgium) ***BAMline***

Magnetron sputter deposition of copper target onto liquids having a low vapor pressure leads to the formation of colloidal solutions of small copper nanoparticles that can oxidize due to reaction with solvent. Using XAFS measurements at Cu-K-edge (8.979 keV) we explore the chemical state of the active species of copper in castor oil and poly(ethylene glycol) methyl ether acrylate solutions.

Atomic relaxations in single-phase Al_x-FeCoNiCr high-entropy alloys

Alevtina Smekhova (Helmholtz-Zentrum Berlin, Germany) ***BAMline***

Element-specific EXAFS spectroscopy in conjunction with reverse Monte Carlo based analysis makes it possible to quantify the differences in atomic relaxations of each 3d constituent existing in the single-phase Al_x-FeCoNiCr high-entropy alloys depending on the crystallographic structure (fcc or bcc). A degree of surface atoms oxidation and magnetic properties are compared for both alloys as well.

XMCD and EXAFS studies of single-phase Mn-rich CrMnFeCoNi high-entropy alloy

Alevtina Smekhova (Helmholtz-Zentrum Berlin, Germany) ***BAMline***

Element-specific X-ray absorption spectroscopy has been applied to probe the magnetic, electronic and structural properties of single-phase fcc-structured Mn-rich CrMnFeCoNi high-entropy alloy on the local scale. The values of magnetic moments, the number of 3d holes, surface oxidation and local ordering including inner relaxations of 3d constituents within a thin film were evaluated.

Modification of surface properties by angle-dependent O_2 plasma treatment of the sustainable polymer polyhydroxybutyrate (PHB)

Lucas Beucher (Uni Koblenz, Germany) ***HE-SGM***

Surface properties of biodegradable PHB are changed by plasma enhanced chemical vapor deposition using O_2 approaching from different angular directions. Results show that this process, previously assumed as cleaning step, changes contact angle, water vapour transmission and the chemical structure depending directly on the angle of plasma incidence and thus extend the range of functions.

Investigating contact primer layers with NEXAFS spectroscopy

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

NEXAFS spectroscopy on extended aromatic hydrocarbons allows to gain insight into their unoccupied electronic states. Here, we apply this technique to F4TCNQ and F6TCNNQ thin films on single- and polycrystalline silver substrates to examine the use of these films as contact primer reducing the contact resistance for subsequently deposited p-type organic semiconductors such as pentacene.

Anchoring of transition metal complexes for small molecule activation on Au(111) surfaces

Kai Uwe Clausen (Christian-Albrechts-Universität zu Kiel, Germany) ***HE-SGM***

Metallic surfaces have the ability to affect adsorbed or covalently bound molecules through electronic interactions, which leads to a change in the intrinsic molecular properties with the effect of activation of small molecules such as CO, O_2, N_2, H_2, N_2O. The functionalization of metal surfaces with well-ordered adsorbates could generate new functional hybrid interfaces to developed new catalytic systems.

Early stages of plasma induced carbon nanowall growth

Eva Kovacevic (Université d'Orléans, France) ***HE-SGM***

Carbon nanowalls (CNWS) have a great potential for a broad range of applications, as e.g. catalyst support for fuel cells, battery electrode materials and sensors. This contribution deals with the plasma assisted growth of CNWs in a low power RF discharge. Special emphasis is put on the early growth stage, which is analysed by means of XPS and angular dependent NEXAFS, AFM and SEM.

Amorphous hydrogenated carbon (a-C:H) layer growth on industrial polycarbonates - Weak interlayer and distinct dehydrogenation

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

Due to its hardness, polycarbonate is used in in many industrial areas (e.g. automotive, data storage). However, some applications are affected by its surface properties that can be adapted by RF PECVD deposition of amorphous hydrogenated carbon (a-C:H) layers. Such layers were deposited in various thicknesses (10–2000 nm) and analyzed with AFM/SEM (morphology) and XPS/NEXAFS (carbon bond states).

Effect of aromatic sidechain of substituted oligoamide self-assembly

Claire Buchanan (La Trobe University, Australia) ***IRIS***

N-acetylated substituted oligoamides form unique nanorods, that further assemble into supramolecular structures. Previously, an oligoamide with tryptophan and lysine sidechains were found to crosslink with Cu(II), forming a metallosupramolecular framework (MFS). Here, tryptophan is replaced with tyrosine and phenylalanine and characterised (IR microscopy, AFM, & SAXS) and assessed for MFS.

Characterization of archaeological glass beads from the ancient Vaccaei culture at the IRIS beamline

Javier Pinto (University of Valladolid, Spain) ***IRIS***

The study of 65 archaeological glass beads found at Pintia (Padilla de Duero, Valladolid, Spain), from different centuries (IV-I BC) and manufacturing, by infrared spectroscopy at the IRIS beamline (BESSY II, Helmholtz-Zentrum Berlin (HZB)) provided evidence about their composition and the alteration procedures of their surfaces, aiming to improve their preservation for future generations.

Status of the IRIS Beamline Microscopy upgrade project

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

Connecting Scales in Vibrational Imaging is a collaborative research project between the Humboldt-Universität zu Berlin and the HZB to upgrade the infrared IRIS beamline microscopy station. The upgrade allows spatial- and polarization-resolved infrared microspectroscopy at and beyond the diffraction limited spatial resolution (micrometer to nanometer scale). Presented here is the status of the upgrade.

In situ imaging of cellulose fibrils orientation in secondary cell walls of Sorghum bicolor

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

Orientation of cellulose microfibrils in plant cell walls was measured in situ by synchrotron polarized FTIR microspectroscopy at IRIS-beamline. Local directionality of the macromolecules was determined at selected spots of the plant cells of different tissues by polarization-dependent measurements. Preferential orientation of cellulose in the plant cell walls is demonstrated.

Induced reduction by H2 exposure at room temperature of ceria ultrathin films grown by atomic layer deposition

Carlos Morales (BTU Cottbus-Senftenberg, Germany) ***KMC-1***

Ceria ultrathin films grown by ALD show an initial Ce3+/Ce4+ mixture that almost entirely re-oxidizes after exposure to ambient conditions. These initial defects allow a weakly reduction at room temperature under 1 mbar of H2, reversible after exposure to ambient conditions. These preliminary results are promising for decreasing the operating temperature of multiple sensing and catalytic devices.

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

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

Photoswitchable crystalline porous frameworks are able to switch between two or more phases upon adsorption of gas molecules, UV-vis irradiation or both stimuli. Herein we present the instrumentation for the comprehensive characterization of photoswitchable MOFs by in situ PXRD, which allow to determine the contribution of each separate stimuli to structural switching.

Time resolved in situ synchrotron X-ray diffraction for structural and reaction mechanism correlation during CO_2 capture on lithium and sodium zirconates

Nadia Gamba (*Comisión Nacional de Energía Atómica,* Argentina) ***KMC-2***

Li-Na zirconates are promising sorbents for CO2 capture at high temperatures with potential application for exhaust gases treatment from hydrocarbon combustion processes. Carbonation/decarbonation was studied in situ by SXRPD measurements from room temperature up to 800 °C under CO_2 flow. Changes in the behaviour of the carbonate phases were observed when using 1 or 0.2 bar CO_2 pressure.

Coupled in-situ GIWAXS and PL investigation of hybrid perovskite semiconductor crystallization from solution to thin film

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

In this work, we study the evolution of MAPbI3 hybrid perovskite from solution to thin film by means of coupled in-situ GIWAXS and PL measurements. The correlation between the optical and structural properties of the intermediate phases formed during the transformation of the crystalline solvate phases into the perovskite phase allows for a simple method for monitoring of material formation.

Crystal structure transitions in $BiMnO_{(3+d)}$: temperature and doping dependence

Vadim Sikolenko (Karlsruhe Institute of Technology, Germany) ***KMC-2***

We present data for temperature dependence of the structure of $BiMnO_{(3+d)}$ with $0 < d < 0.14$. We have observed a transition from none polar monoclinic structure to another monoclinic and than to polar orthorhombic structure with an increase of temperature and oxygen content. Experiment has been performed at the KMC-2 beamline.

Catalysis research with operando-XAS at KMC-3

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

The status of experiments using operando-XAS approaches (time- and energy-resolved rapid-scan XANES and EXAFS) in a wide energy range (2-14 keV) for analysis of catalytic materials using in-situ electrochemistry or light-excitation of samples is presented and recent and planned instrumental improvements are discussed.

Transient negative thermal expansion in HgTe/CdTe heterostructures by heating transverse phonons

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

We investigate the transient negative thermal expansion of semimetallic HgTe and semiconducting CdTe by using synchrotron-based time-resolved X-ray diffraction. At T = 20 K, far below the Debye temperature of both materials, the selective optical excitation of the HgTe top layer with an ultrashort near-infrared laser pulse leads to a rapid expansion of HgTe that is followed by a long lasting contraction.

Accessing the disorder-disorder transitions in MOFs by synchrotron single-crystal X-ray diffraction

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

Metal-Organic Frameworks are crystalline porous solids, promising for gas storage, separation and catalysis applications. As in other crystalline solids, structural disorder often influences or even determine the properties of the solid. Herein we studied repeatable switching transitions between distinct disorder states in DUT-8(Ni) framework using data collected at MX beamlines of BESSY-II.

Chasing a wild goose - amorphous calcium sulfate and "forbidden" phase transitions

Tomasz Stawski (Bundesanstalt für Materialforschung und -prüfung, Germany) ***mySpot Beamline***

Calcium sulfate minerals (i.e. gypsum, anhydrite and bassanite) are ubiquitous on Earth. The current consensus is that the formation of phases involves a nanosized precursor and intermediate amorphous phases. A general question arises, if all three phases of CaSO form through a similar non-classical pathway, which would involve the same common precursor amorphous phase?

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

Andrey Sokolov (Helmholtz-Zentrum Berlin, Germany) ***Optics Beamline***

Multilayer-coated blazed gratings (MLBG) are very promising optics for high flux grating monochromators for the tender X-ray range (1 - 4 keV) which is difficult for commonly used single coated diffraction gratings or crystal monochromators. The work presents the results on MLBG developments as combination of theory, numerical simulations and prototype structures efficiency measurements.

Unveiling the electronic state interplay at organic DBP/4P-NPD exciton blocking interfaces in organic solar cells

Mariam Ahmad (University of Southern Denmark) ***PM4***

Ultra-thin 4P-NPD films have been demonstrated to function as efficient exciton blocking layers in organic solar cells, resulting in up to 24 % better device performance. In this work, we have conducted an all in-situ photoelectron study to uncover the full energy level alignment at the interface between DBP (electron donor) and 4P-NPD to understand the mechanisms behind the improved device performance.

Charge Transfer from Organic Molecules to Molybdenum Disulfide: Influence of the Fluorination of Iron Phthalocyanine

Katharina Greulich (Eberhard Karls Universität Tübingen, Germany) ***PM4***

Adsorption of molecules is a promising way to tune the electronic structure of molybdenum disulfide (MoS_2). We study interface properties between MoS_2 and differently fluorinated iron phthalocyanines using (angle-resolved) photoelectron spectroscopy and X-ray absorption spectroscopy. For non-fluorinated iron phthalocyanine, charge transfer from the molecule to the substrate is observed.

Organic radical-based magnetic monolayers on gold surfaces

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

We investigate thin films of exceptionally chemically stable radical self-assembled monolayers based on the perchlorotriphenylmethyl (PTM) radical by using X-ray based techniques. The results clearly indicate that (mono)layers of PTM radical derivatives have the necessary stability to withstand working conditions in devices.

Crystalline and amorphous calcium carbonate as structural components of the Calappa granulata exoskeleton

Maria Katsikini (Aristotle University of Thessaloniki, Greece) ***RGBL Dipole***

Raman and NEXAFS spectroscopies are applied to investigate the C. granulata crab exoskeleton. The main Raman peak of CaCO3 reveals the presence of calcite and amorphous calcium carbonate (ACC). In the Ca L3,2-edge NEXAFS spectra, the peak separation due to crystal field splitting is directly related to the ACC percentage. Finally, C K-edge spectra provide the extent of the exoskeleton calcification.

Oxygen K-edge RIXS study of spin-orbit induced excitonic quasiparticles in Sr_2RhO_4

Valentin Zimmermann (Max-Planck-Institute for Solid State Research, Germany) ***U41-PEAXIS***

We investigate spin-orbit coupling (SOC) related phenomena in the correlated metal Sr_2RhO_4 using resonant inelastic x-ray scattering (RIXS) at the O K-edge, which is sensitive to hybridized states between Rh 4d-orbitals and O ligand 2p-orbitals. The RIXS spectra reveal dispersive modes that are associated with spin-orbit entangled states, underlining the importance of SOC in 4d-electron materials.

Study of metal-carboxylate complex derived from Pinus elliotti resin applied as antibacterial and antifungal pigment in home paints

Carla Bittencourt (University of Mons, Belgium) ***U41-TXM***

Besides the antibacterial and/or antiviral properties of pigments, colour and stability are important characteristics often associated to the oxidation state of the doping metal atom. We investigated pigments of metal complex with carboxylate binder (Zn, Mn, Fe, Co, Ni or Cu), derived from Pinus elliotti var. elliotti. NEXAFS edges, anti-bacterial and anti-viral activities will be presented.

Expanding Liquid-Jet Photoelectron Spectroscopy to Free-Flowing Planar Surfaces

Dominik Stemer (Fritz-Haber-Institut, Germany) ***U49-2_PGM-1***

Here, we ent our design for the generation of a liquid flat jet. Additionally, we demonstrate flat-jet photoelectron spectroscopy (FJ-PES), a new subset of liquid-jet PES, confirm that turbulent mixing within the first jet leaf is negligible in the near-surface region, and finally, report the generation of an unexpectedly large electric potential gradient of 100 kV/m across the liquid flat jet.

History dependent skyrmion and domain formation in van der Waals magnet Fe_3GeTe_2

Max Birch (Max Plank Insitute for Intelligent Systems, Germany) ***UE46_MAXYMUS***

Recently, observations of skyrmions in the 2D magnet Fe_3GeTe_2 have been reported, opening application possibilities. Control of the magnetic state requires knowledge of the sample's history-dependence, which remains unexplored in 2D magnets. We utilise real-space imaging to map phase diagrams of an exfoliated FGT flake, revealing the complex, history-dependent emergence of the skyrmion states.

Demonstrating optical-pump-x-ray probe experiments at 50 MHz repetition rate on a solid-state sample

Kathinka Gerlinger (Max-Born-Institute, Germany) ***UE46_MAXYMUS***

We present a pump-probe experiment carried out with the infrared pump laser newly installed at the MAXYMUS x-ray microscope at BESSY II. We were able to record time-resolved images of ferrimagnetic thin films at 50 MHz repetition rate at a fluence of 3.2 mJ/cm² without sample damages, which to our knowledge is the highest repetition rate achieved in an ultrafast demagnetization experiment, so far.

Controlling Magnetic Skyrmion Nucleation and Motion

Lisa-Marie Kern (Max-Born-Institute, Germany) ***UE46_MAXYMUS***

Magnetic skyrmions can be generated current-induced or optically. While the nucleation mechanisms are different, both suffer from a stochasticity in the spatial distribution of skyrmions. In view of applications, a controllable localization of the skyrmion's nucleation site is required. Nanopatterning of the magnetic anisotropy landscape using He^+-ions provides a platform for enhanced control of skyrmions.

Unravelling the Effect of superficial Rh depletion on shallow d-states of Gallium-Rhodium Liquid Metal Alloys

Tzung-En Hsieh (Helmholtz-Zentrum Berlin, Germany) *UE48_EMIL*

The chemical and electronic structure of supported GaRh alloys has been studied to reveal the active phase in supported catalytically active liquid metal solutions (SCALMS). XPS and UPS of in-system prepared GaRh alloys with Rh concentrations from 1% to 80% on silicon oxide substrate show narrowing of Rh 4d derived valence states for alloys with Rh concentration <5%.

MYSTIIC at EMIL: New Scanning Transmission X-Ray Microscope (STXM) is open to users

Tianxiao Sun (Helmholtz-Zentrum Berlin, Germany) *UE48_EMIL*

A new Scanning Transmission X-ray Microscopy (STXM) with focus on the development of complex sample environment for in-situ/operando characterization of catalytic and electrochemical processes has started operation and been open to friendly users at the Energy Materials in situ Lab (EMIL) since September 2021. And it has been first time in regular call for proposals for general users.

The relation of structure sensitivity and doping of ceria [(111) vs (100)] for CO_2 hydrogenation

Emilia Pozarowska (BTU Cottbus-Senftenberg) *UE49_PGM SMART*

Alloying CeOx with samarium reduces the near-surface region of (100)-oriented CeOx islands, whereas their bulk and (111)-oriented islands retain their Ce4+ original state. This behavior highlights the structure sensitivity for this process and constitutes a promising result with a high impact on heterogeneous catalysis.

Optical formation and annihilation of skyrmions

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

The use of skyrmions in memory devices requires non-volatile manipulation. We investigate the conditions for deterministic formation and annihilation of skyrmions in thin ferromagnetic films. Both experimentally and in simulation, we observe that a combination of single and multiple laser pulses can write or erase skyrmions. Our experiments are performed by XMCD-PEEM with in-situ laser excitation.

XAS study of electronic structure and oxidation states of manganese atoms in cold gas-phase $Mn_2O_x(H_2O)^{n+}$ clusters.

Olesya Ablyasova (Helmholtz-Zentrum Berlin, Germany) *UE52_PGM Nano cluster trap*

Photosystem II, with its active center a $CaMn_4O_5$ cluster coordinated by H_2O molecules, is essential for O_2 production in nature. Due to the challenging sample production of such complex, the composite Mn_2O_{x+} clusters were chosen as an investigation object. We initiated an X-ray absorption spectroscopy study of these clusters with attached H_2O to investigate the structure changes and Mn oxidation state.

Leveraging XAS for Operando Investigation of mfCVD

Benjamin May (Forschungszentrum Jülich, Germany) ***UE56-1_SGM***

We have applied XAS to MgFe2O4 grown by magnetically functionalised CVD. Applying a magnetic field during film growth has a significant impact on the magnetisation of the grown film, and point to mfCVD as a promising technique for the preparation of materials with engineered magnetic properties. To elucidate the growth process, we are retrofitting the XMCD chamber with CVD capabilities for operando studies.

CORE LAB Quantum Material

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

We describe the offers of the core lab “quantum materials”:

(1) powder and single crystal preparation
(2) material analysis: stoichiometry, phase purity, single crystallinity etc.
(3) orientation, shaping and crystal mount for any experiment requirement
(4) magnetisation, resistivity, specific heat, thermal transport as function of temperature and field

4D Wavelength-Resolved Neutron Tomography for Polycrystalline Materials

Khanh Van Tran (Helmholtz-Zentrum Berlin, Germany)

Neutron wavelength-selective tomography has been acquired for Dual-phase steel under torsional deformation. The neutron Bragg-edge based method is applied for stainless steel with TRIP that shows the phase transformation from austenite to martensite under strain. The 4D data sets (3D + spectral) of plastically deformed TRIP steel were used for analyzing the crystalline phase fractions.

OTHER TOPICS *BEAMLINE*

Hidden details in teeth revealed by complementary X-ray techniques

Leona Bauer (Helmholtz-Zentrum Berlin, Germany) ***BAMline***

Within the DFG project 'IXdent', first results have been achieved on 2D µXRF and X-ray refraction radiography measurements as well as combined 3D confocal µXRF and µXCT investigations at the interface between filling and bovine tooth tissue. The benefit of multiple analytical techniques and the combination of structural and elemental analysis will be demonstrated.

Spectroscopic studies of on-surface synthesis of chiral graphene nanoribbons on Au(788)

Igor Chunin (Trinity College Dublin, Ireland) ***HE-SGM***

We investigate graphene nanoribbons on-surface synthesis explicitly including temperature-dependent growth on vicinal Au(788) studied by STM, synchrotron based core level XPS of the C1s and Br3d core levels and NEXAFS studies at the C1s edge. Comparison is made between the simulated and observed high-resolution spectra. NEXAFS data presented reveals the orientation of GNRs and correlates with STM images.

Synchrotron far-infrared spectroscopy as a tool for studying historical pigments: new insights, prospects and limitations

Hartmut Kutzke (University of Oslo, Norway) ***IRIS***

Whilst mid-infrared spectroscopy (MIR) is a well-established method to investigate pigments remains the far-infrared (FIR) region widely unstudied. FIR allows identification of pigments undetectable by MIR and provides in other cases valuable additional information to MIR data. Our project is a systematic study on historical pigments, their components and alteration products.

All-optical switching behaviour of a GdFe ferrimagnet by using single and dual laser pulses

Rahil Hosseinifar (Freie Universität Berlin, Germany) ***UE49_PGM SPEEM***

Ferrimagnetic $Gd_{26}Fe_{74}$ thin films with out-of-plane magnetization were excited by single and dual linearly polarized 100-fs infrared laser pulses. Single laser pulses reversed the magnetization, while local deviations from this deterministic behaviour were observed close to magnetic domain walls. More effective switching is achieved for double-pulse excitation with < 1 ps pulse separation.

Reactivity and Passivation of Fe-NCs on h-BN/Rh(111)

Natalie Waleska (Friedrich-Alexander-Universität, Germany) ***UE56-2_PGM-2***

Fe nanocluster arrays (Fe-NCs) formed in the pores of h-BN/Rh(111) were studied by in situ HR-XPS using CO as a probe molecule. CO dissociation was observed on the as-prepared Fe-NCs. For the C and O precovered Fe-NCs a passivation of the catalytic activity was found as a result of adsorption site blocking, allowing for the determination of the most active sites of the Fe-NCs.

Structural and compositional characteristic variations of archaeological marbles

Ioannis Siouris (Democritus University of Thrace, Greece) ***CoreLab X-ray***

XRD patterns of ancient marble samples from Pistiros Greece, exhibit apart from the expected major calcite and dolomite phases, additional distinguishable CaMg carbonate phases with characteristic mineralogical variations. Rietveld analysis allowed a preliminary mineral quantification. The determined parameters may be correlated to the origin of the marbles and provide an extra tool in provenance studies.

Understanding solid formation via in situ spectroscopy

Monica Distaso (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

The implementation of in situ spectroscopy is an effective strategy to understand the formation mechanism of solid materials. A customized reactor allows for up to 4 simultaneous and complementary in situ measurements including photoluminescence, UV/Vis, FTIR and Raman spectroscopy, dynamic light scattering (DLS). An overview on metal oxides, mesocrystals, metal-organic-framework will be shown.

New experimental opportunities at HZB: laboratory spectrometers for 3D elemental imaging and soft NEXAFS spectroscopy

Ioanna Mantouvalou (SyncLab Berlin, Germany)

By combining measurements in the lab with investigations at large scale facilities, both the users as well as the instrumentalists benefit. From the spring call 2022, HZB facilitates access to perform experiments at the BLiX in the frame of SyncLab through the Gate system. X-ray fluorescence spectrometers for 3D elemental imaging as well as a twin arm NEXAFS spectrometer can be accessed for joint projects.

Less is more - crafting your message to a target audience

Antonia Rötger (Helmholtz-Zentrum Berlin, Germany)

Information overload is a stressful experience. Time and attention are scarce. Can cognitive psychology help to design better posters? What would be the best poster design from their point of view? At the poster session, I want to get into conversation with researchers about what they expect from poster presentations, what works and what does not.

Diversity@HZB

Jennifer Schevardo (Helmholtz-Zentrum Berlin, Germany)

The HZB is the first non-university research institution in Germany to have undergone the Stifterverband's diversity audit. For more than a year, we have been working together to develop and implement ideas to make HZB a place where all employees can contribute and develop, regardless of their life phase, cultural background, gender, physical ability, field of expertise etc. It is only a start.

PTB LABORATORY AT BESSY II

Applying a model-free parameterization for reconstruction of nanostructures from grazing incidence X-ray flourescence measurements

Anna Andrle (Physikalisch-Technische Bundesanstalt, Germany)

Periodic SiO2 gratings are element-sensitively reconstructed using a method based on GIXRF measurements. The experimental data can be simulated by calculating the XSW field using a model-free parameterization with B-splines of the nanostructure. A Bayesian optimizer is used for efficient sampling of the spatial distribution of the material composition of the nanostructures.

Intermediate plans for a new soft X-ray beamline at the PTB laboratory

Richard Ciesielski (Physikalisch-Technische Bundesanstalt, Germany)

After successful 20 years of operation, PTB's soft X-ray beamline at BESSY II is now being redesigned and updated to extend its capabilities and to adapt for future challenges. We discuss the merits and drawbacks of the less common choice of a constant focus factor (cff) below 1 in the plane grating monochromator regarding the achievable energy resolution, spot size, beam divergence and imaging properties.

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 SAXS pattern of a single particle freeing us from using tricky analytic form factors.

Quantitative and qualitative characterisation of trace elements in pancreatic and pancreatic carcinoma 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.

Background correction of SAXS data using CT

Christian Gollwitzer (Physikalisch-Technische Bundesanstalt, Germany)

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 a SAXS signal for every voxel of the sample interior. We use SAXS-CT on fluid-filled glass capillaries to retrieve SAXS curves without the background signal from the capillary wall.

PTB LABORATORY AT BESSY II

Reference-free grazing incidence X-ray fluorescence applied to the validation of calibration samples to be used for a quantitative analysis of airborne particulate matter

Yves Kayser (Physikalisch-Technische Bundesanstalt, Germany)

Reference-free X-ray spectrometry allows for an independent validation of quantification results and can as such be applied to the analysis of calibration samples. Such samples are needed for assessing unknown instrumental factors of total reflection X-ray fluorescence instrumentation in order to allow for a quantitative investigation of samples stemming from air pollution monitoring campaigns.

Dimensional nanometrology with angle resolved X-ray scattering in the EUV spectral range

Leonhard Lohr (Physikalisch-Technische Bundesanstalt, Germany)

X-ray scattering in the EUV spectral range can be used for measuring critical dimensions of nanostructured semiconductor surfaces. A single image covers the q-space if the beam incidence angle reaches 15 deg and if the beam spot can be brought close to the area detector. We present a small and compact measurement setup which allows smooth scans over a large angular range with small beam spot size.

Investigation of halide perovskite precursor solutions with small-angle X-ray scattering (SAXS)

Ana Palacios Saura (Helmholtz-Zentrum Berlin, Germany)

Precursor solutions of the photovoltaic absorber materials (MA,FA)Pb(I,Br)$_3$ in different GBL:DMF solvent ratios were investigated using SAXS to understand the influence of the solvent in the crystallization path. We show first results demonstrating that changing the solvent ratio affects the agglomerates in solution, indicating a strong solvent influence at the onset of the crystallization state.

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

Qais Saadeh (Physikalisch-Technische Bundesanstalt, Germany)

The determination of optical constants regarding three tantalum-cobalt binary alloys is carried in the spectral range 8 nm - 22 nm. Utilizing a Bayesian-based Markov-Chain Monte-Carlo approach, the optical constants are determined from angle-dependent reflectivity data collected from sputtered thin films using a synchrotron radiation source.

Alignment strategy for a von Hamos Spectrometer with a full cylinder geometry

Kai Schüler (Physikalisch-Technische Bundesanstalt, Germany)

One of the key points in the operation of a crystal spectrometer is the alignment of its components to the desired geometry in order to optimise the instrumental response and ensure a robust calibration of the energy axis. Here, the strategy for optimising the physical source position and the crystal orientation for von Hamos spectrometer with full cylinder crystals will be presented.

PTB LABORATORY AT BESSY II

Vacuum-Compatible Magnetic Sample Environment for in-situ SAXS/WAXS Measurements on Magnetic Nanoparticles

Dieter Skroblin (Physikalisch-Technische Bundesanstalt, Germany)

A vacuum-compatible magnetic sample environment for X-ray scattering experiments has been developed. The design is based on a water-cooled electromagnetic coil setup and is aimed to provide a magnetic flux of up to 900 mT at the sample position. The magnetic field is applied in order to align or arrange magnetic nanoparticles. The scattering patterns are collected as 2D images on area detectors.

Database of optical constants in the soft X-ray spectral range

Victor Soltwisch (Physikalisch-Technische Bundesanstalt, Germany)

The determination of fundamental optical parameters is essential for the development of new optical elements such as mirrors, gratings, or photomasks. Especially in the extreme ultraviolet (EUV) and soft X-ray spectral range, the existing databases for the refractive indices of many materials and compositions are insufficient or are a mixture of experimentally measured and calculated values.

Traceable analysis of individual nanoscaled objects by means of X-ray fluorescence with high spatial resolution

André Wählisch (Physikalisch-Technische Bundesanstalt, Germany)

This work presents the transfer of SI-traceable XRF to the submicron and nano-scale where structures of similiar lateral extent than the excitation beam size are investigated. In addition to determining the total elemental mass, a numerical algorithm based on the Monte Carlo technique can be utilised to reconstruct spatial parameters such as length, height and orientation of nano objects.

Simultaneous dimensional and analytical characterization of ordered nanostructures

Nils Wauschkuhn (Physikalisch-Technische Bundesanstalt, Germany)

The complexity of today’s 3D nanostructures necessitates new metrology techniques. Here the method of grazing exit X-ray fluorescence will be demonstrated, with which an ensemble of regularly ordered nanostructures can be characterized simultaneously with sub-nm discrimination for crucial dimensional and analytical parameters. It is non-destructive and compatible with typically sized test fields.

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 2021 [00:01] - 09. December 2021 [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 legislative term 2022/23 are

Volodymyr Bon	Technische Universität Dresden, Germany
Justin Wells	University of Oslo, Norway

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

The members of the current election committee are

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

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.

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Name/name		
Abteilung/department		
Straße/street		
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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.

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

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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 August 2022 to December 2022.

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

http://hz-b.de/gate

DEADLINE
March 1st, 2022