HZB Helmholtz Zentrum Berlin

11th JOINT BER II AND BESSY II USER MEETING

Dec. 4-6, 2019

Keynote Lecture:
Gert Weber (U Greifswald and HZB)

Public Lecture:
Volker Quaschning, Scientists for Future (HTW Berlin)
Clara Mayer, Fridays for Future
Bernd Rech (HZB)

Invited Talks:

Bernd Smarsly (U Giessen)
Ingo Manke (HZB)
Peter Smeibidl (HZB)
Sebastian Wintz (PSI and HZDR)
Wolfgang Kuch (FU Berlin)
Ute Cappel (KTH)
Artiom Magomedov (KTU)
Janina Kneipp (HU Berlin)
Martin Hennecke (MBI Berlin)
Travis Jones (FHI Berlin)
Phil Mason (Czech Academy of Sciences)
Simon Krause (U of Groningen)
Astrid Brandt (HZB)

- **Neutron Instrumentation Day**
- **Science Day**
- **Synchrotron Instrumentation Day**
- **Young Scientists Sessions**
- **Vendor Exhibition**
- **Poster Session**

„MATERIALS METROLOGY“ - Joint HZB-PTB Satellite Workshop to the User Meeting 2019:

1st in the BESSY III Foresight Workshop Series.
December 3rd to 4th, lunch-to-lunch, at the Wilhelm-Conrad-Röntgen Campus in Berlin-Adlershof.

Lise-Meitner-Campus (Berlin-Wannsee), WISTA and Wilhelm-Conrad-Röntgen Campus (Berlin-Adlershof)

http://hz-b.de/um2019

Helmholtz-Zentrum Berlin

für Materialien und Energie GmbH

Wilhelm-Conrad-Röntgen Campus:

BESSY II

Albert-Einstein-Str. 15
12489 Berlin
tel +49 30 8062 - 0
photons(at)helmholtz-berlin.de

Lise-Meitner Campus:

BER II

Hahn-Meitner-Platz 1
14109 Berlin
tel +49 30 8062 - 0
neutrons(at)helmholtz-berlin.de

https://www.helmholtz-berlin.de/

Dear Users and Friends,

Welcome to the 11th Joint BESSY II and BER II User Meeting 2019.

This year we look gratefully back to 46 years of Neutron Research at our Neutron Source BER II at which forefront scientific research has been conducted. A very special word of thanks goes to the vivid user community which till the very end is actively and vibrantly making use of BER II as well as to all members of HZB staff keeping the facility and the instruments running. We are glad that most of the instruments of BER II look forward to new homes, at MLZ and other sources in Europe and elsewhere, and will serve the BER II user community at these facilities as old friends. With a proud and a crying eye we therefore solemnise the farewell to BER II, expressing our sincere gratitude to all users and colleagues, who contributed to the success of BER II.

An average of more than 100 publications per year documenting the achievements of Neutron Research in Berlin shall be highlighted by the following examples from magnetism research, battery research and cultural heritage. A first glimpse of Dirac strings and magnetic monopoles in spin ice $Dy_2Ti_2O_7$ has been discovered (Science 326 (2009), 411), neutron tomography has revealed hidden facts of Li anode in Cycled Lithium-Oxygen Batteries (ACS Energy Letters 4 (2019), 306), and insights were given in the genesis of Jan Steens painting “As the old one sings, so the young ones pipe” (Nuclear Instruments & Methods in Physics Research A 651 (2011), 273).

Our Photon Source BESSY II celebrated 20 years of operation last year. To stay at the forefront as a world leading soft X-ray source our facility is under continuous development and constant improvement. To secure reliable operation over the coming years an investment programme for upgrading components from the source to the end stations has been started in 2019. In this context, we would also like to thank our users for proposing once again exciting projects in response to the “Verbundforschung” – the BMBF programme to support universities to develop innovative instrumentation and new research methods at large scale facilities, of which 10 proposals were successful and will be funded by the BMBF. “Verbundforschung” as a tool only comes to life by you, the BESSY II user community, your ideas and projects, and we are deeply grateful for your engagement and look very much forward to the new experimental capabilities as well as your future project suggestions.

Of course all these developments require time, sometimes even shut-down periods. This year’s shut down was in many respects very successful. All three cryogenic insertion devices are installed and operational. In particular, we would like to stress that the CPMU 17, which extends the photon energy range of the EMIL facility into the tender X-ray range, can now be tuned over its entire design range.

The BESSY II facility, however, is only the horse to run a race – the jockey wins the medal! And there are many outstanding scientific results achieved by you, the BESSY II user community, worth celebrating. With more than 500 published results per year, however, it is almost impossible to do justice to everyone by mentioning just a few highlights, but we kindly invite you to visit the HZB Newsroom and subscribe to our Newsletters.

En route for defining the long term future of synchrotron radiation based research in Berlin, we have recently launched the BESSY III Conceptual Design Report Phase. This facility shall build on the strengths of BESSY II and its user community and will consequently be optimized for X-ray spectroscopy based research in the soft to tender X-ray photon energy range, expanding on HZB's longstanding expertise in source, optics and instrument development. To identify the needs of the current BESSY II and future BESSY III user community, the series of foresight workshops will be continued, the Materials Metrology Workshop taking place as a satellite meeting of this User Meeting being the first of the meetings foreseen for the coming years.

This year's User Meeting will again underline the broad variety of scientific fields addressed by the experiments realized by you at the HZB facilities. Particular highlights are the Keynote Lecture on "Structural basis of enzymatic plastic degradation - *en route* to a sustainable circular economy" by Gert Weber, the Panel Discussion on the Climate Challenge with representatives from Fridays for Future and Scientists for Future, and the bestowal of the Ernst-Eckhard-Koch Prize for an outstanding doctoral thesis and the Innovation Award on Synchrotron Radiation.

Thank you for joining the User Meeting! We look very much forward to fruitful discussions, inspiring new ideas, a vivid exchange and future collaborations.

A cordial welcome to you! Enjoy the meeting.

Sincerely

Prof. Dr. Bernd Rech
Scientific Director

Prof. Dr. Jan Lüning
Scientific Director

Contents

Wednesday, December 4th, 2019:
Young Scientists and Neutron Day

Lise-Meitner Campus
Hahn-Meitner-Platz 1
14109 Berlin

13:00 – 16:00	**Registration**		(LMC-Foyer and Café Jahn)
13:30 – 15:15	**Young Scientists Session**	*(Chair: Susan Schorr)*	(Lecture Hall)
13:30	*Jan Lüning (HZB)* **Opening**		
13:45	*Margarita Russina (HZB)* **NEAT**		
14:00	*Leonie Heinze (TU Braunschweig, Germany)* **High magnetic field studies on atacamite, $Cu_2Cl(OH)_3$, a model compound for the S = 1/2 sawtooth chain**		
14:15	*Heiko Trepka (MPI Stuttgart, Germany)* **Critical magnetic fluctuations in Ca_2RuO_4 studied by neutron triple-axis spectroscopy**		
14:30	*Stephan Allenspach (PSI, Switzerland)* **Dimensionality of $BaCuSi_2O_6$ studied by Neutron Diffraction on HFM/EXED**		
14:45	*Galina Gurieva (HZB)* **Cu/Zn disorder vs. solar cell efficiency: the $Cu_2ZnSn(S_xSe_{1-x})_4$ monograin case**		
15:00	*Anderson Ferreira Sepulveda (Federal University of ABC, Brazil)* **Using SANS to show morphological structure of drug delivery nanomaterials**		
15:15 – 15:45	**Coffee Break**		(Café Jahn)
15:45 – 18:00	**Farewell from BER II**	*(Chair: Jan Lüning)*	(Lecture Hall)
	Jan Lüning (HZB) **Introduction**		
	Astrid Schneidewind (Komitee Forschung mit Neutronen) **Welcoming Words**		
	Bernd Smarsly (Universität Giessen, Germany) **20 years of neutron scattering – insights into nanostructured SiO_2 and carbon**		
	Ingo Manke (HZB) **Science with Neutrons and Tomography**		
	Peter Smeibidl (HZB) **Neutron experiments under extreme conditions: Sample Environment**		
	Sparkling Wine Reception		
18:00 – 22:00	**Farewell Party: Poster Session & Buffet**		(LMC-Foyer and Café Jahn)

Thursday, December 5th, 2019:
Science Day

Wilhelm-Conrad-Röntgen Campus
Albert-Einstein-Str. 15
Rudower Chaussee 17
12489 Berlin

09:00 – 16:00	**Vendor Exhibition**	WISTA Centre
08:30 – 16:30	**Registration**	WISTA Centre
15:00 – 18:30	**Poster Set-up (BESSY II - Experimental Hall)**	
09:30 – 09:40	**Opening** *Bernd Rech (HZB)*	Bunsen Auditorium
09:40 – 10:10	**Keyote Lecture** *(Chair: Manfred Weiss)* *Gert Weber (Universität Greifswald/HZB, Germany)* **Structural basis of enzymatic plastic degradation - *en route* to a sustainable circular economy**	
10:10 – 10:20	*Tribute to Sergey Troyanov for 2000 solved structures at MX@BESSY II*	
10:20 – 10:50	**Coffee Break and Vendor Exhibition**	WISTA Centre
10:50 – 12:30	**Oral Presentations I** *(Chair: Marcus Bär)*	Bunsen Auditorium
10:50	*Sebastian Wintz (PSI, Switzerland and HZDR, Germany)* **Spin textures and spin waves as seen by X-ray microscopy**	
11:10	*Wolfgang Kuch (Freie Universität Berlin, Germany)* **Manipulating magnetic domains by single ultrashort laser pulses**	
11:30	*Ute Cappel (KTH Royal Institute of Technology, Sweden)* **Stability of perovskite materials for solar cells investigated with photoelectron spectroscopy**	
11:50	*Artiom Magomedov (Kaunas University of Technology, Lithuania)* **Self-Assembled Hole Transporting Monolayer for Highly Efficient Perovskite Solar Cells**	
12:10	*Janina Kneipp (Humboldt Universität zu Berlin, Germany)* **Plasmonic nanoparticle probes in cells: Insights from X-ray tomography**	
12:30 – 13:30	**Lunch Break**	(Canteens on site)

13:30 – 15:10	**Oral Presentations II** *(Chair: Christian Papp)*	Bunsen Auditorium
13:30	*Martin Hennecke (Max-Born-Institut Berlin, Germany)* **Angular Momentum Flow During Ultrafast Demagnetization of a Ferrimagnet**	
13:50	*Travis Jones (Fritz-Haber-Institut Berlin, Germany)* **The Electronic Structure of Iridium Oxyhydroxides during Electrocatalytic Oxygen Evolution**	
14:10	*Phil Mason (Czech Academy of Sciences, Czech Republic)* **Almost the Weirdest Thing in the Universe Meets BESSY**	
14:30	*Simon Krause (University of Groningen, Netherlands)* **X-rays and neutrons shed light on negative gas adsorption mechanism in flexible metal-organic frameworks**	
14:50	*Astrid Brandt (HZB)* **Unveiling Hidden Secrets: Cultural Heritage Studies at HZB – A Selection**	
15:10 – 15:20	**Report from the User Committee and the ESUO**	Bunsen Auditorium
15:20 – 15:50	**Coffee Break and Vendor Exhibition**	WISTA Centre
15:50 – 17:00	**Bestowal of Prizes: Friends of Helmholtz-Zentrum Berlin e.V.** *(Chair: M. Richter)*	Bunsen Auditorium
17:00 – 18:30	**Public Lecture**	Bunsen Auditorium
	Panel and General Discussion on the Climate Challenge **Volker Quaschning, Scientists for Future (HTW Berlin)** **Clara Mayer, Fridays for Future** **Bernd Rech (HZB)**	
18:30 – 20:00	**Poster Session**	(BESSY II Experimental Hall)
20:00	**"Green" Buffet** **(sponsored by the companies participating in the vendor exhibition)**	(BESSY II Foyer)

Friday, December 6th, 2019 :
Young Scientists and Synchrotron Day

Wilhelm-Conrad-Röntgen Campus
Albert-Einstein-Str. 15
Rudower Chaussee 17
12489 Berlin

08:30 – 10:00	**Registration**	WISTA Centre
09:00 – 12:30	**Vendor Exhibition**	WISTA Centre
09:00 – 10:30	**Synchrotron Session** *(Chair: Christian Jung)*	Bunsen Auditorium
09:00	*Bernd Rech/Jan Lüning (HZB)* **Welcome**	
09:10	*Jan Lüning (HZB)* **BESSY II: Photon Science**	
09:30	*Andreas Jankowiak (HZB)* **Accelerator - Operation, Development and BESSY VSR & bERLinPro**	
09:50	*Ioanna Mantouvalou (Technische Universität Berlin)* **From synchrotron into the lab and back**	
10:10	*Jens Viefhaus (HZB)* **BESSY II – beamline maintenance and modernization**	
10:30 – 10:40	**General Discussion**	Bunsen Auditorium
10:40 – 11:00	**Coffee Break and Vendor Exhibition**	WISTA Centre
11:00 – 12:30	**Young Scientists Session** *(Chair: Carolin Schmitz-Antoniak)*	Bunsen Auditorium
11:00	*Katrin Fürsich (MPI FKF Stuttgart, Germany)* **Interface Induced Structural and Magnetic Reconstructions in $NdNiO_3$ Thin Film Structures**	
11:15	*Heidi Therese Hillier (University of Tromsø, Norway)* **Characterizing Enzymes in the ectoine biosynthesis pathway**	
11:30	*Alice Dupont Juhl (University of Southern Denmark, Denmark)* **Analysis of Nieman Pick C2 Protein in Regulation of Intracellular Membrane Transport by Combined and Correlative Fluorescent and Soft X-ray Microscopy**	
11:45	*Maxim Rabchinskii (Ioffe Institute St Petersburg, Russian Federation)* **Graphene chemical derivatives and functionalized carbon nanodots: from synthesis to applications**	
12:00	*Raphael Jay (Universität Potsdam, Germany)* **Charge distributions of iron photosensitizers probed with L-edge spectroscopies**	
12:15	*Ludvig Kjellsson (Uppsala University, Sweden)* **X-ray absorption spectroscopy of the N_2^+ molecular cation**	
12:30	**Poster Prize and Closing Remarks**	
12:40	**Traditional curried sausage**	WISTA Centre

Abstracts of the Young Scientists Session - Neutron Day

Wednesday, 4th of December

High magnetic field studies on atacamite, $Cu_2Cl(OH)_3$, a model compound for the $S = ½$ sawtooth chain

L. Heinze[1], V. Vapf[2], X. Ding[2], C. Corvalán Moya[2], F. Weickert[2], M. Jaime[2], N. Harrison[2], M. Reehuis[3], J.-U. Hoffmann[3], M. Bartkowiak[3], O. Prokhnenko[3], R. Feyerherm[3], D. Menzel[1], A. U. B. Wolter[4], K. C. Rule[5], S. Süllow[1]

1 Institut für Physik der Kondensierten Materie, Germany
2 National High Magnetic Field Laboratory, USA
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
4 Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden, Germany
5 Australian Nuclear Science and Technology Organisation ANSTO, Australia

As indicated by band structure calculations, the natural mineral atacamite, $Cu_2Cl(OH)_3$, represents a model compound of the $S = ½$ sawtooth chain with an antiferromagnetic coupling J_1 along the chain and a second antiferromagnetic coupling J_2 within the sawteeth with $J_2/J_1 \sim 1/3$ [1]. By means of thermodynamic studies as well as neutron diffraction measurements, we have extensively characterized the magnetic phase diagram of atacamite: In low magnetic fields and below $T_N = 8.9$ K a long-range ordered antiferromagnetic state with a magnetic propagation vector of $\mathbf{q} = (½\ 0\ ½)$ is present [2]. By means of neutron diffraction, we have fully determined the magnetic structure below T_N [1].

Further, we have probed the intermediate and high magnetic field region of the magnetic phase diagram by means of pulsed magnetic field magnetostriction and magnetization measurements. Here, we have found a magnetization plateau at $M = ½\ M_{sat}$ along all three principal crystal axes, and which is entered for magnetic fields $\mu_0 H > 31.5$ T for $H \,||\, b$ axis [1].

A static high magnetic field neutron scattering experiment at the HFM/EXED instrument at HZB allowed us to investigate the magnetic phase diagram of atacamite in further detail. By measuring the integrated intensity of selected magnetic reflections up to 26 T ($H \,||\, b$ axis), we find that the antiferromagnetically ordered state is suppressed in magnetic fields that are significantly lower than the magnetization plateau field. This implies that the antiferromagnetic phase is distinct from the plateau phase at finite temperatures. It suggests that the plateau phase is of an exotic nature.

[1] arxiv:1904.07820 [cond mat.str el]
[2] Physica B 536, 377 (2018)

Critical magnetic fluctuations in Ca_2RuO_4 studied by neutron triple-axis spectroscopy

H. Trepka[1], T. Keller[1], M. Hepting[1], M. Krautloher[1], J. Porras[1], J. Xu[2], K. Habicht[2], B. Keimer[1]

1 Max-Planck-Institut für Festkörperforschung, Germany
2 Helmholtz-Zentrum für Materialien und Energie, Germany

We report on high-resolution linewidth measurements of critical antiferromagnetic fluctuations in Ca_2RuO_4 (CRO), performed at the neutron triple-axis spectrometer FLEXX at BER II. CRO hosts a complex interplay between magnetic and electronic correlations and exhibits a novel type of soft magnetism with strong single-ion anisotropy, and 'Higgs' amplitude fluctuations in the spin-wave spectrum as revealed by recent neutron experiments [1]. However, the nature of the electronic order in CRO above the magnetic ordering temperature (TN ~ 110K) is still under debate and the emergence of an exotic spin-nematic or an orbitally ordered state have been suggested [2,3]. Since the magnetic fluctuations in proximity to T_N are fundamentally related to the nature of the magnetism, with the magnetic order parameter possibly coupling to the electronic states, our investigation of the critical magnetic scattering might help to clarify the type of the electronic order in CRO.

[1] Nat. Phys. 13, 633 (2017)
[2] Phys. Rev. Lett. 122, 057203 (2019)
[3] Phys. Rev. Lett. 95,136401 (2005)

Dimensionality of $BaCuSi_2O_6$ studied by Neutron Diffraction on HFM/EXED

S. Allenspach[1,2], P. Puphal[1], A. Biffin[1], J. Lass[3], C. Niedermayer[1], G.S. Tucker[4], M. Bartkowiak[5], A. Gazizulina[5], X. Liu[5], O. Prokhnenko[5], B. Normand[1], N. Laflorencie[6], F. Mila[7], E. Pomjakushina[1], Ch. Rüegg[1,2]

1 Paul Scherrer Institut (PSI), Switzerland
2 University of Geneva, Switzerland
3 University of Copenhagen, Denmark
4 ISIS Facility, United Kingdom
5 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
6 CNRS and Université de Toulouse, France
7 Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

The quantum magnet $BaCuSi_2O_6$ consisting of stacked spin dimer bilayers, undergoes an unconventional dimensional reduction from 3D to 2D close to the quantum critical point [1]. Mechanisms for this dimensional reduction were proposed based on inter-bilayer frustration originating from antiferromagnetic intra-bilayer interaction parameters. Ab-initio calculations indicate ferromagnetic intra-bilayer interaction parameters rendering frustration impossible [2]. In addition to previous measurements of $BaCuSi_2O$ [3], we have performed neutron spectroscopy experiments on $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ [4] using the new neutron spectrometer CAMEA at SINQ. Furthermore, we have measured the phase boundary of the Bose Einstein Condensate phase in $BaCuSi_2O_6$ using neutron diffraction under extreme conditions on HFM/EXED at HZB up to magnetic fields as high as 26T.
Our results demonstrate ferromagnetic intra-bilayer interaction parameters with at least three different dimer types in $BaCuSi_2O_6$ and only one dimer type in $Ba_{0.9}Sr_{0.1}CuSi_2O_6$. We conclude that the existence of different dimer types in $BaCuSi_2O_6$ leads to the observed unconventional critical scaling. We modeled the critical properties by Quantum Monte Carlo simulations which are in excellent quantitative agreement with previous measurements and tested the predictions by high-field magnetic neutron diffraction.

[1] Nature 441, 617 (2006)
[2] PRL 112, 107202 (2014)
[3] submitted (2019)
[4] PRB 93, 174121 (2016)

Cu/Zn disorder vs. solar cell efficiency: the $Cu_2ZnSn(S_xSe_{1-x})_4$ monograin case

G. Gurieva[1], A. Franz[1], K. Muska[2], K. Ernits[2], S. Schorr[1,3]

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
2 crystalsol OÜ, Estonia
3 Freie Universität Berlin, Germany

Kesterite-type based thin films solar cell technologies are mainly based on polycrystalline absorber layers. A promising low cost alternative technology uses kesterite monograins (single crystals of 50-100 µm size) which are fixed in a polymer matrix to form a flexible solar cell [1]. It is agreed in literature that large band tailing observed in Cu-based kesterite-type semiconductors causes voltage losses limiting the efficiency of kesterite-based devices [2]. The Cu/Zn disorder (Cu_{Zn} and Zn_{Cu} anti-sites in Cu-Zn planes at z=¼ and ¾), which is always present in these compounds [3], is discussed as a possible reason for band tailing [4].
The experimental determination of the order parameter Q which is a quantitative measure of the degree of Cu/Zn disorder [5] requires a differentiation between the isoelectronic cations Cu^+ and Zn^{2+}. An in depth analysis of neutron diffraction data provides information on the cation distribution in the crystal structure allowing the determination of type and concentration of intrinsic point defects including a distinction between Cu and Zn [3]. On the other hand neutron diffraction requires large sample volumes, thus kesterite monograins offer the unique possibility to correlate structural disorder in kesterite-type absorbers with solar cell performance parameters.
We will present a detailed structural investigation of CZTSSe monograins based on neutron powder diffraction experiments. The order parameter Q representing the Cu/Zn disorder as well as the occurring intrinsic point defects have been determined. We will present the influence of the purity of the starting material (copper) as well as small changes in the chemical composition on the Cu/Zn disorder resulting in different power conversion efficiencies of the respective devices.

[1] www.crystalsol.com
[2] Sol. En. Mat. Sol. Cells 172, 149 (2018)
[3] J. Appl. Phys. 123, 161519 (2018)
[4] Appl. Phys. Lett. 105, 112106 (2014)
[5] Phys. Stat. Sol. B 253, 1890 (2016)

Using SANS to show morphological structure of drug delivery nanomaterials

A. Ferreira Sepulveda[1], M. K. D. D. Franco[2], F. Yokaichiya[3], D. R. de Araújo[1]

1 Federal University of ABC (UFABC), Brazil
2 Energetic and Nuclear Research Institute (IPEN), Brazil
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Nanomaterials based on organic formulations have shown relevant potential for controlled drug release, mainly due low toxicity, low costs, and some have ability to change their material characteristics under temperature. Small-angle scattering techniques can help to characterize molecular assembly of drug delivery systems and then we can study the structural role over drug release behaviour. Moreover, Small-angle neutron scattering (SANS) allows to analyse how temperature affects nanostructure organization, which contributs to material improvement and development of new drug delivery formulations when is combined with other physical-chemical techniques, such as rheology, dynamic light scattering, differential scanning calorimetry and scanning electron microscopy.
SISLIBIO is a Brazilian research group that develops new pharmaceutical and cosmetic formulations based on thermosensitive intelligent gels, combining synthetic and natural polymers. For some years, the group has done SANS measurements at Helmholtz-Zentrum Berlin for different hydrogel and organogel compounds. In 2019, the group studies one hydrogel formulation (based on poloxamer and hyaluronic acid carrying bupivacaine and ropivacaine), and other different kind of organogels, made of poloxamer and lipids combination. A software has been developed by SISLIBIO for SANS and SAXS analysis of these materials.

Abstracts of the Farewell from BER II Session - Neutron Day

Wednesday, 4th of December

20 years of neutron scattering – insights into nanostructured SiO_2 and carbon

B. M. Smarsly[1]

1 Justus Liebig University, Germany

My contact with the neutron source at "Hahn-Meitner-Institut" began in 1999, when we performed an in-situ experiment, combining small-angle neutron scattering (SANS) with physisorption of nitrogen, utilizing a setup (SANSADSO) developed by Dr. Hoinkis, together with the group of Prof. Findenegg. The contrast matching between condensed nitrogen and SiO_2 allows for studying the mechanisms of nanopore filling and emptying. Having the chance to measure two of my own nanoporous SiO_2 materials was definitely a tremendous boost for my PhD thesis and also my scientific career.[1] Fortunately, the cooperation with Dr. Astrid Brandt and Dr. Dirk Wallacher, who developed the DEGAS setup, helped my group to perform further in-situ SANS experiments and provided very important insights into the different fundamental mechanisms of condensation and evaporation of fluids in confined space. [2,3] For instance, we were able to prove a special emptying mechanism ("cavitation") for defined nanopores in SiO_2 being connected to the outside through much smaller connecting pores, which helped to verify theory. Furthermore, we really appreciate several beamtimes for small- and wide-angle neutron diffraction experiments (WANS) on carbons. These data helped us to unravel the microstructure of so-called "non-graphitic" carbon, i.e. the disordered graphene structure, in relation to the nanoporosity in such carbons.[4]
Thanks to the great support of the HZB team these neutron-based results certainly were of great support for my scientific career! Also, several PhD students of my group had the unique chance to get excellent data for their PhD works and unparalleled experience, both in science and in personal relationships with HZB coworkers.
Thanks BER, for many outstanding moments!

[1] J. Phys. Chem. 105, 831 (2001)
[2] Langmuir 23(9), 4724 (2007)
[3] Langmuir 25(21), 12670 (2009)
[4] Carbon 141, 169 (2019)

Science with Neutrons and Tomography

I. Manke[1], N. Kardjilov[1], A. Hilger[1], H. Markötter[1,2], T. Arlt[1,2], M. Osenberg[2], A. Tengattini[4,5], C. Tötzke[3], J. Banhart[1,2]

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
2 Technische Universität Berlin, Germany
3 University Potsdam, Germany
4 Institut Laue-Langevin, Grenoble, France
5 Laboratoire 3SR, Université Grenoble Alpes, France

This talk will focus on some major achievements related to the neutron imaging instrument CONRAD I+II/V7 [1-7] at Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) and will provide an outlook on the future of the new CONRAD-III/NeXT instrument after transfer of CONRAD I+II/V7 to the ILL in Grenoble. Recent applications of neutron imaging techniques in both materials research and fundamental science will be illustrated by examples selected from different areas.
One of the most important catalysts for the further improvement of neutron imaging techniques is the rapidly increasing demand for in-situ and operando investigations of materials and devices that are used for energy supply, such as batteries, electrolyzers, hydrogen storage materials and fuel cells [1]. Here, the properties and the operation characteristics of the related materials and devices are often closely connected to the distribution and movement of light elements such as lithium and hydrogen. Neutrons have the unique property to be highly sensitive to such light materials, even if these are embedded in a metallic material or in a closed metallic environment that strongly absorbs X-rays. These unique properties make neutrons perfectly suited probes for research on materials that are used for energy storage and conversion. Moreover, the wave properties of neutrons can be exploited to perform phase-contrast and dark-field imaging experiments. Their magnetic moment allows for resolving magnetic properties in bulk samples. Therefore, neutron imaging allows one to analyze phenomena in materials research not accessible by other existing experimental techniques as will be illustrated with some examples [1,6]. First know-how transfer [9] to ILL resulted in two world records: the fastest tomography and the currently highest spatial resolution [1,8].

[1] Mat.Today 21, 6 (2018)
[2] Nat.Comm 1, 125 (2010)
[3] Nat.Phys. 4, 399 (2008)
[4] Adv.Mat. 26, 4069 (2014)
[5] Nat.Comm. 9, 4023 (2018)
[6] Mat.Today 14, 6 (2011)
[7] PRL 101, 123902 (2008)
[8] Opt.Ex. 27, 20, 28640 (2019)
[9] Nat.Comm. accepted (2019)

Neutron experiments under extreme conditions: Sample Environment

P. Smeibidl[1], K. Kiefer[1], M. Meissner[1], D. Wallacher[1]

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

A historical overview on 25 years of sample environment for the BER II is presented. Enclosed are technical details of standard sample environment, which was used during this time almost without technical modifications as well as the continuous development of special and extreme sample environment for low temperatures and high magnetic fields.
New fields of science, changing requirements from the users and growing international collaborations changed the field of work.
Goals and achievements are reported.

Neutron News 6, 3 (1995)
Neutron News 12, 3 (2001)
EEE Transactions on Applied Superconductivity 26, 4, (2016)

Abstract of the Keynote Lecture - Science Day

Thursday, 5th of December

Structural basis of enzymatic plastic degradation - *en route* to a sustainable circular economy

G. Weber[1]

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Synthetic polymers (plastics) are indispensable for our daily life - we appreciate their diverse material properties and durability. At the same time, high production rates and in particular chemical stability have turned them into a global environmental burden. Uncontrolled disposal has led to their accumulation in the environment - as larger debris and virtually omnipresent when fragmented to microplastics. Current recycling methods cover only a fraction of plastics and still suffer from their dependence on crude oil or extensive energy consumption. Recently, enzymes were recognized as a promising alternative. Enzymatic polymer recycling enables the breakdown of plastics to the very building blocks at low temperatures. Hence, this technology has the potential to establish crude-oil free circular economies with a minimal carbon-loss for nearly one third of all plastics. One example is the extremely durable and popular polyester polyethylene terephthalate (PET) which amounts to about 18% of all synthesized polymers[1]. In 2016, a group of Japanese researchers discovered a bacterium that grows and partially feeds on PET employing two enzymes, PETase and MHETase[2].
Initially, *Ideonella sakaiensis* PETase converts PET to mono-(2-hydroxyethyl) terephthalate (MHET). MHETase subsequently hydrolyzes MHET to terephthalate and ethylene glycol which are the building blocks for a new round of PET synthesis. However, the enzyme's activities are still too low for applications on an industrial scale. Structural characterization of PETase and MHETase bound to their ligands and structure-based bioengineering are essential to improve both enzymes until economic viability is reached. We have obtained the first high-resolution structure of active apo-MHETase and MHETase bound to a non-hydrolyzable MHET analog and thus set the basis for semi-rational bioengineering approaches. In the light of our structure-based mapping of substrate requirements as well as initial activity improvement, we anticipate MHETase to be a valuable resource to further advance enzymatic plastic degradation[3]. Our research sets the basis for strategies to target other polyesters such as the emerging bio-based polyethylene furanoate (PEF), as well as polyamides or polyurethanes leading to a circular and sustainable economy for synthetic polymers.

References
[1] Sci. Adv. 3, e1700782 (2017)
[2] Science 351, 1196–9 (2016)
[3] Nat. Commun. 10, 1717 (2019)

Abstracts of the Oral Presentations - Science Day

Thursday, 5th of December

Spin textures and spin waves as seen by x-ray microscopy

S. Wintz[1]

1 Max-Planck-Institut für Intelligente Systeme, Germany

The investigation of spin-wave phenomena, also referred to as *magnonics*, plays an important role in present condensed matter research [1] [Fig. 1]. This holds true, in particular, as spin waves are seen as signal carriers for future spintronic information processing devices, with a high potential to outperform present charge-based technologies in terms of energy efficiency and device miniaturization. Yet a successful implementation of magnonic technology will require the usage and control of spin waves with nanoscale wavelengths.

Here, I will show that ferromagnetic spin textures in metallic systems can be used as nanoscale spin-wave emitters and wave guides. In particular, topological spin vortex cores prove to act as efficient and tunable generators for sub-100 nm waves [2,3] [Fig. 2(a,b)], while domain walls can be utilized as quasi one-dimensional channels for spin-wave propagation and routing [4] [Fig. 2(c)]. The underlying spin dynamic processes were directly imaged by using time-resolved x-ray microscopy at the Maxymus endstation of BESSY II.

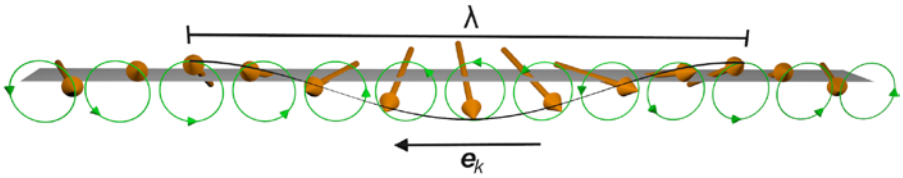


Figure 1: Schematics of a propagating spin wave [3].

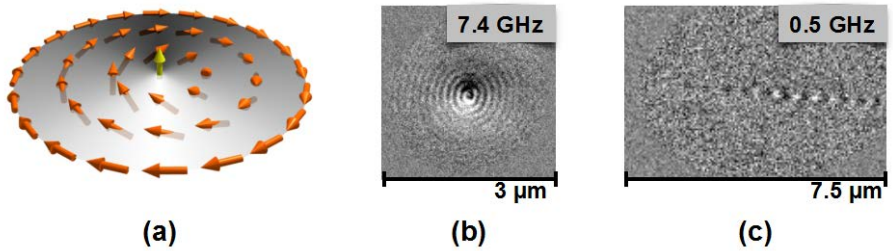


Figure 2: (a) Schematics of a spin vortex. (b) Spin-wave emission from a vortex core. (c) Domain wall as 1D spin-wave channel.

[1] Nat. Phys. 11, 453 (2015)
[2] Nat. Nanotech. 11, 948 (2016)
[3] Phys. Rev. Lett. 122, 117202 (2019)
[4] Nat. Nanotech. 14, 328 (2019)

Manipulating magnetic domains by single ultrashort laser pulses

Y. A. Shokr[1,2], O. Sandig[1], M. Erkovan[3], B. Zhang[1], M. Bernien[1], A. A. Ünal[4], S. Valencia[4], F. Kronast[4], U. Parlak[5], J. Vogel[6], W. Kuch[1]

1 Freie Universität Berlin, Germany
2 Helwan University, Egypt
3 INESC-Microsystems and Nanotechnologies, Portugal
4 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
5 Gebze Technical University, Turkey
6 Université Grenoble Alpes and Institut Néel (CNRS), France

Moving magnetic domain walls, i.e., the boundaries between oppositely magnetized regions, in a magnetic film just by light is of high interest with respect to potential applications in computing technology and data storage. Here we investigate by means of space-resolved x-ray magnetic circular dichroism photoelectron emission microscopy (XMCD-PEEM) the effect of single focused ultrashort (100 fs) infrared laser pulses on the domain configuration in ultrathin magnetic films. We observe that in epitaxial Co/Cu/Ni trilayers on a Cu(001) single-crystal substrate, single-shot fs laser pulses can induce significant depinning and motion of domain walls, leading to a local switch of the magnetization direction. The distance traveled by an individual domain wall after one pulse in zero external magnetic field—up to several hundred nanometers—is much longer than what a domain wall could possibly move during the electronic excitation of the system assuming realistic domain-wall velocities. We explain our results by a two-step model of laser-induced depinning and successive thermal motion of domain walls.
In a Co/$Fe_{75}Gd_{25}$ bilayer, the magnetic domain walls experience a force in the gradient of the laser pulse away from the center of the pulse, which can be used to move domain walls optically into a certain direction. We discuss this effect in terms of spin waves traveling in the transient lateral lattice-temperature gradient from the hotter to the colder part of the sample and being reflected at the domain walls, which exerts a torque on the domain wall moving it towards the colder side. The time scale of the transient temperature change by the laser pulse matches the times necessary for the observed domain-wall displacements. This possibility to steer domain walls by ultrashort laser pulses might open new avenues for writing magnetic information.

PRB 99, 214404 (2019)
PRB 94, 054414 (2016)

Stability of perovskite materials for solar cells investigated with photoelectron spectroscopy

U. Cappel[1], S. Svanström[2], A. García Fernández[1]

1 KTH Royal Institute of Technology, Sweden
2 Uppsala University, Sweden

Solar cells have a great potential in replacing fossil fuels in electricity generation, if requirements of low production costs can be met. In the last years, lead halide perovskites have drastically changed the solar cell research field due to their ease of synthesis and high power conversion efficiencies, which now reach over 25%. The materials have developed from methylammonium lead iodide ($MAPbI_3$) to structures containing anion (e.g. Br^- and I^-) and cation (e.g. formamidinium, MA, Cs^+ and Rb^+) mixtures. The use of mixed structures can enhance both solar cell efficiencies and stability. For commercial applications, a high chemical and structural stability of perovskites themselves as well as of the interfaces with contacting materials is needed to achieve long-term solar cell operation without a loss in efficiency. It is therefore of high importance to understand how the exact composition of the perovskite influences stability.

In this presentation, I will show how we have used photoelectron spectroscopy to determine the photo-stability of different perovskite active materials under visible laser illumination [1,2]. Measurements presented here were carried out at the LowDosePES beamline at BESSY II, where a low photon flux is combined with a highly efficient spectrometer [3]. This enables us to study the electronic structure of perovskites without any X-ray degradation. Instead, we were able to follow changes in our materials induced by visible illumination. By carrying out such measurements on perovskite materials with different compositions, we followed the degradation in perovskite materials and found that the addition of Cs^+ significantly enhances the photo-stability of the active material. Finally, I will show results of in-situ studies of the interface formation and interface degradation of a perovskite active layer with metal contacts.

[1] ACS Appl. Mater. Interfaces 9, 34970 (2017)
[2] J. Mat. Chem. A 6, 22134 (2018)
[3] J. Electron Spectrosc. Relat. Phenom. 224, 68 (2018)

Self-Assembled Hole Transporting Monolayer for Highly Efficient Perovskite Solar Cells

A. Magomedov[1], A. Al-Ashouri[2], E. Kasparavičius[1], M. Jošt[2], T. Malinauskas[1], S. Albrecht[2], V. Getautis[1]

1 Kaunas University of Technology, Lithuania
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Over the last decade, the rapid progress of the perovskite-based solar cells (PSCs) led to the record efficiencies of over 25%, approaching that of the best Si-based technologies (26.7%). One of the important constituents of the PSCs is a hole transporting material (HTM). Recently it was shown, that a commonly used doping procedure is leading to the intrinsic instability of the HTM layer [1]. Moreover, the prices of the most popular HTMs Spiro-OMeTAD (~500 €/g) and PTAA (~2000 €/g) are very high, which in a combination with the low stability serve as one of the main obstacles on the way towards successful commercialization of PSCs.
In the search for an ideal HTM, it is important to avoid above mentioned drawbacks. One of the ways to exclude the use of the dopants is to reduce the thickness of the HTM layer. However, this comes at the cost of the reduced open-circuit voltage, due to the incomplete coverage of the substrate [2].
In our work, we have proposed to use self-assembled monolayers, as a way towards the robust formation of the ultimately thin layer, with the thickness of a single molecule. For the proof of concept, carbazole-based HTM, with a phosphonic acid functional group, was synthesized. p-i-n PSC with this molecule showed a promising performance of over 17 % [3].
Upon further optimization of the structure, over 21% efficiency was achieved, which is currently the best result for the devices, that are not using dopants and/or interlayers. In addition, the world record was achieved for the CIGS/PSC monolithic tandem device, reaching 23.26% efficiency on an active area of 1 cm^2 [4].

[1] J. Mater. Chem. C 6, 8874, (2018)
[2] Energy Environ. Sci. 10, 1530 (2017)
[3] Adv. Energy Mater 8, 1801892 (2018)
[4] Energy Environ. Sci. 12, 3356 (2019)

Plasmonic nanoparticle probes in cells: Insights from X-ray tomography

J. Kneipp[1], D. Drescher[1], V. Živanović [1], T. Büchner[1], G. P. Szekeres[1], S. Werner[2], P. Guttmann[2], G. Schneider[2], S. Seifert[3], C. Arenz[1]

1 Humboldt-Universität zu Berlin, Germany
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
3 Kiel University, Germany

Plasmonic nanoparticles hold great promise in many analytical, theranostic, and biotechnological applications. We develop different types of optical nanoprobes that function based on the high local optical fields of gold and silver nanostructures, specifically by obtaining surface-enhanced Raman scattering (SERS) spectra from the compartments of eukaryotic cells. While a SERS spectrum can tell us precise details about the molecules that interact with the nanostructures inside the cells, e.g., the interaction with drugs and their targets, also the the sub-cellular localization of the nanostructures and their potential effects on cellular ultrastructure must be understood. Therefore, we conduct experiments by cryo-X-ray tomography. As will be discussed, this enables data sets that allow a 3D volume rendering of both cellular organelles and the nanoparticle aggregates of different sizes in intact cells of different cell lines. The distribution and shape of the intracellular nanoprobes depend on the duration of incubation and the specifics of the experiment. Examples will be shown of nanoprobes that are used for monitoring enzyme activity in live cells and the spectroscopic information that they deliver, of nanostructures of different sizes and materials, and of composite structures that can serve as multifunctional vehicles.

ACS Nano 13(8), 9363 (2019)
Nanoscale Advances 1, 2937 (2019)
Analyst 141(17), 5096 (2016)

Angular Momentum Flow During Ultrafast Demagnetization of a Ferrimagnet

M. Hennecke[1], I. Radu[1], R. Abrudan[2], T. Kachel[2], K. Holldack[2], R. Mitzner[2], A. Tsukamoto[3], and S. Eisebitt[1,4]

1 Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Germany
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
3 Nihon University, Japan
4 Technische Universität Berlin, Germany

The use of light pulses to manipulate and control the magnetic order parameter on the fundamentally limiting time and length scales is an important quest in modern magnetism. Recent studies of ferrimagnetic GdFeCo alloys have revealed an ultrafast laser-induced magnetization reversal mediated by a transient ferromagnetic-like state [1]; such switching was purely thermally driven without the need of any other external stimulus [2]. However, the ultrafast angular momentum transfer from and into the spin system during demagnetization and switching events as well as the role and dynamic contributions of spin and orbital moments still remain unclear [3].
Here, we report on time- and element-resolved soft x-ray magnetic circular dichroism (XMCD) measurements performed at the FemtoSpeX slicing facility of BESSY II synchrotron, which reveal the angular momentum flow during femtosecond laser-induced demagnetization of a ferrimagnetic GdFeCo alloy. A magneto-optical sum rules analysis of the fs-XMCD data allows us to monitor and disentangle the dynamics of elemental spin and orbital moments at Fe and Gd sites. For our experimental conditions (≈100% demagnetization), we observe the absence of angular momentum exchange between the two antiferromagnetically coupled sublattices. Furthermore, we observe that angular momentum is not redistributed between spin and orbital moment at the Fe and Gd sites within the experimental time resolution (130 fs) and conclude that the orbital moment is not acting as a bottleneck for the angular momentum transfer from spin moment to the lattice, in agreement with theoretical prediction [4]. The complete transfer of spin and orbital angular momentum to the lattice occurs during the first hundreds of femtoseconds of the demagnetization process.

Original publication: M. Hennecke et al., Physical Review Letters 122, 157202 (2019)

[1] Nature 472, 205 (2011)
[2] Nature Communications 3, 666 (2012)
[3] Handbook of Magnetic Materials 26, 291 (2017)
[4] Physical Review Letters 115, 217204 (2015)

The electronic structure of iridium oxyhydroxides during electrocatalytic oxygen evolution

T. E. Jones[1], H. N. Nong[2,3], L. J. Falling[1], A. Bergmann[1], M. Klingenhof[3], H. P. Tran[3], C. Spöri[3], R. Mom[1], J. Timoshenko[1], G. Zichittella[4], A. Knop-Gericke[1,2], S. Piccinin[5], J. Pérez-Ramírez[4], B. Roldan Cuenya[1], R. Schlögl[1,2], P. Strasser[3], D. Teschner[1,2]

1 Fritz-Haber-Institute of the Max-Planck-Society, Germany
2 Max-Planck-Institute for Chemical Energy Conversion, Germany
3 Technische Universität Berlin, Germany
4 ETH Zurich, Switzerland
5 Consiglio Nazionale delle Ricerche CNR-IOM, Italy

Electrocatalysts provide access to useful chemistries for chemical energy conversion, but understanding the origin of their catalytic performance remains challenging. The underlying understanding of electrocatalytic chemistry is largely phenomenological and is assumed to be at odds with that familiar from traditional gas-phase catalysis. We show this assumption is not always valid. In particular, by combining *operando* potentiodynamic X-ray absorption spectroscopy and *ab initio* computation we demonstrate that an important class of electrocatalytic reaction, oxygen evolution on iridium oxyhydroxides, can be described as a traditional catalytic reaction. We find the role of the electrochemical bias is to create electron deficient oxygen species on the catalyst surface. The chemistry taking place on this surface is then controlled by the concentration of these species in a traditional catalytic manner rather than directly by the applied potential. This gives rise to a linear relationship between the free energy of activation and degree of surface oxidation, that can be probed electrochemically.

[1] J. Phys. Chem. C123, 9146 (2019)
[2] Nature Catal. 1, 841 (2018)
[3] Chem. Sci. 8, 2143 (2017)
[4] Chem. Sci. 7, 6791 (2016)
[5] Phys. Chem. Chem. Phys. 18, 2292 (2016)

Almost the Weirdest Thing in the Universe Meets BESSY

P. Mason[1]

1 Czech Academy of Sciences, Czech Republic

Electrons are weird particles! Almost all the stuff that surrounds us is made up of electrons bound by nuclei. To get an electron that isn't bound to a nuclei typically requires very high energies. About a hundred years ago, some guy found a way that you could actually get a stable solution of electrons- not bound by atomic nuclei! Electrons just sit there in a solution.... of liquid ammonia. If you add certain alkali metals to liquid ammonia, you first of all get a blue solution of solvated electrons, which then turns into a metallic gold solution at high concentrations. That solution of lithium in a non-conductor (ammonia) conducts electricity better than silver! This is the story of what happened when this liquid met BESSY.

X-rays and neutrons shed light on negative gas adsorption mechanism in flexible metal-organic frameworks

S. Krause[1, 2], V. Bon[2], J. Evans[2], D. M. Többens[3], A. Franz[3], D. Wallacher[3], S. Kaskel[2]

1 University of Groningen, The Netherlands
2 Technische Universität Dresden, Germany
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Crystalline porous solids are in general perceived as mechanical robust and applied in various technologies. However, an increasing number of so-called soft porous crystals are reported to demonstrate structurally defined softness initiated by external stimuli. The presence of intrinsic porosity and the resulting high surface area allows these systems to exhibit a rich host-guest chemistry which can initiate and stimulate structural transformation in the porous solid. Recently, we discovered that a metal-organic framework (MOF) undergoes volumetric contraction by over 50% initiated by the interaction with methane molecules at 111 K.[1] The subsequent reduction in pore volume causes expulsion of methane molecules previously present in the expanded pores and an unusual negative slope occurs in the adsorption isotherm. The so-called negative gas adsorption (NGA) occurs at a very defined pressure due to the cooperative nature of the structural transition which was investigated by *in situ* X-ray diffraction. By shortening and elongation of the struts in the framework backbone a series of structurally related MOFs was established which were characterized for their NGA properties.[2] In these materials the adsorption mechanism was refined using *in situ* neutron diffraction on CD_4 loaded solids allowing to refine gas distribution on the molecular level. From these findings we derive condensation in the larger cavities and the correlating capillary stress as the underlying driving force for the transition of NGA and demonstrate a second material capable of this unusual phenomenon.

[1] Nature 532, 348–352 (2016)
[2] Nature Commun. 10, 3632 (2019)

Unveiling Hidden Secrets: Cultural Heritage Studies at HZB – A Selection

A. Brandt[1]

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Many ancient artifacts keep their most precious secrets well hidden beneath the surface. While the outside mostly offers a view on craftsmanship and general purpose, the inside might reveal information on for example production techniques, the origin of the used materials or the artisan himself. More interesting, looking underneath the surface might even answer the question of ‚original or fake'. Unveiling these hidden secrets is a great challenge for anyone involved. Since maintaining the integrity of the cultural heritage artifact is of highest priority, non-invasive methods of investigation are the means to an end.

The talk will present a selection of examples for studies on cultural heritage artifacts that have been conducted at the Helmholtz-Zentrum Berlin für Materialien und Energie over the last two decades using lab-source X-rays, synchrotron radiation, neutrons and ion beam experimental techniques.

Abstracts of the Young Scientists Session - Synchrotron Day

Friday, 6th of December

Interface Induced Structural and Magnetic Reconstructions in $NdNiO_3$ Thin Film Structures

K. Fürsich[1], Y. E. Suyolcu[1], M. Bluschke[1,2], E. Schierle[2], M. Hepting[1], Z. Zhong[1], Y. Wang[1], G. Cristiani[1], G. Logvenov[1], E. Weschke[2], P. Hansmann[1,3], P.A. van Aken[1], M. Minola[1], E. Benckiser[1], B. Keimer[1]

1 Max Planck Institute for Solid State Research, Germany
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
3 Max Planck Institute for Chemical Physics of Solids, Germany

Transition metal oxide (TMO) heterostructures are a versatile platform for the stabilization of novel electronic, magnetic, and crystallographic phases in proximity to interfaces. In particular, the heteroepitaxy between different perovskite materials enables the manipulation of the lattice degrees of freedom in the constituent materials, due to the necessity of octahedral connectivity across interfaces.
Here we study the rare-earth nickelates $RNiO_3$, a prototypical TMO system, using resonant x-ray scattering techniques available at BESSY II and other large scale synchrotron facilities. We focus on the $NdNiO_3$ compound, where we observed several magnetic and structural reconstructions. First, we discuss the magnetic properties, where we found a crossover from non-collinear to collinear spin structure as a function of layer thickness. This crossover manifests itself in the spin dynamics and ordering temperature [1, 2, 3]. Second, we exemplify how electronic correlations can be tailored by structural modifications. Specifically, we use resonant elastic x-ray scattering in combination with transmission electron microscopy [4] and DFT calculations to study the enhanced bond-order for a particular substrate orientation.
The demonstration of controlled creation of phases opens a new route to tune material properties in heterostructures for future applications in functional devices.

[1] Phys. Rev. X 8, 031014 (2018)
[2] Phys. Rev. B 99, 165124 (2019) - Editors' Suggestion
[3] Nat. Phys. 14, 1097 (2018)
[4] Adv. Mater. Interfaces (2017)

Characterizing Enzymes in The Ectoine Biosynthesis Pathway

H. T. Hillier[1], B. Altermark[1], I. Leiros[1]

1 UiT The Arctic University of Norway, Norway

We aim to characterize enzymes associated with the biosynthesis of a small organic compound called ectoine, by doing structural and functional studies. Ectoine belongs to a group of molecules known as osmolytes, which are small organic compounds that are actively accumulated in, amongst others, bacterial cells to protect them against environmental stress. Ectoine has many possible biotechnological applications, for example, it can protect cells against changes in temperature and osmolarity but also against drying and freezing, it has high water-retaining abilities, and is shown to have a stabilizing effect on proteins. Our group aims to characterize the three-dimensional structure and biochemical properties of enzymes associated with the biosynthesis of ectoine, to help design better producers of ectoine and interesting variants of either ectoine or other interesting compounds associated with the biosynthesis pathway.

Analysis of Nieman Pick C2 Protein in Regulation of Intracellular Membrane Transport by Combined and Correlative Fluorescent and Soft X-ray Microscopy

A. Dupont[1], F. W. Lund[1], M. L. V. Jensen[1], M. Szomek[1], G. K. Nielsen[2], C. W. Heegaard[3], P. Guttmann[4], S. Werner[4], J. McNally[4], G. Schneider[4], D. Wüstner[1]

1 University of Southern Denmark, Denmark
2 University of Aarhus, Denmark
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
4 University of Copenhagen, Denmark

Cholesterol constitutes an essential part of membranes in mammalian cells. The cell can either synthesize the cholesterol *de novo* or take it up from low density lipoprotein (LDL) particles. Cholesterol from both LDL particles and the plasma membrane gets trapped in late endosomes and lysosomes (LE/Lys) of Niemann Pick Type C diseased cells, which lack functional Niemann Pick C2 (NPC2) protein. NPC2 protein works together with NPC1 protein in LE/Lys to transfer cholesterol out of these organelles. However, how cholesterol is transferred from the LE/Lys to other organelles and how it is efflux from the cell is still not completely clear.
Using fluorescent microscopy combined with cryo-Soft X-ray Tomography (cryo-SXT), we have studied NPC2 protein mediated cholesterol export from LE/Lys.
We have used skin fibroblasts from NPC2 lacking patients as a model system to study efflux of plasma membrane derived sterol from LE/Lys. By quantitative fluorescence microscopy we showed that dehydroergosterol, a weakly fluorescent analogue of cholesterol, became trapped in LE/Lys from where it can slowly efflux from NPC2 lacking fibroblasts. This process was strongly accelerated upon internalization of bovine NPC2 protein. From cryo-SXT we visualized membrane contact sites (MCS, tethered proximity between two membranes, usually in the range of 10-80 nm) between endosomes and other organelles resembling potential routes of intracellular cholesterol transfer. With correlative fluorescent and cryo-SXT we imaged extracellular vesicles containing TopFluor-cholesterol, a green fluorescent analogue of cholesterol, and fluorescent NPC2 protein. We suggest that release of such vesicles resembles a potential route of cholesterol efflux from cells. Cryo-SXT allowed us to visualize the delicate membranes of vesicles without any additional labeling and provided us the resolution required for imaging MCSs, all in 3D.

[1] Nat. Rev. Mol. Cell. Biol. 9, 2 (2008)
[2] Lipid Insights 8, 1 (2015)
[3] Chem. Phys. Lipids 213 (2018)
[4] Traffic 15, 12 (2014)
[5] Nature Commun. 10, 1 (2019)
[6] Submitted, Traffic (2018)

Graphene chemical derivatives and functionalized carbon nanodots: from synthesis to applications

M. K. Rabchinskii[1], S. A. Ryzhkov[2], D. A. Kurdyukov[1], D. A. Eurov[1], M. V. Baidakova[1,2], V. V. Shnitov[1], D. A. Kirilenko[1,2], D. Y. Stolyarova[3], S. I. Pavlov[1], P. N. Brunkov P.N.[2]

1 Ioffe Institute, Saint-Petersburg, Russia
2 ITMO University, Saint-Petersburg, Russia
3 NRC Kurchatov Institute, Moscow, Russia

In the past years the field of nanocarbon materials has been expanding with appearance of new chemical derivatives of graphene and carbon nanodots. Hereby we present our results on the synthesis, study and application of the set of functionalized graphenes (FGs) and carbon nanodots (CNDs). Functionalized graphenes, namely carboxylated (C-xy), carbonylated (C-ny) and aminated (Am) graphenes, were obtained via photochemical and liquid-phase chemical modification of graphene oxide [1,2], whereas functionalized CNDs were synthesized via template method [3]. By the means of synchrotron radiation techniques on the base of Russian-German Laboratory at synchrotron BESSY II (Berlin) chemical composition and specific features of the obtained materials have been discovered. C-xy graphene is demonstrated to contain up to 11 at.% of carboxyls and exhibit the restored sp^2-conjugated network, although arrays of 20-50 nm holes are formed during the modification. Despite its perforated structure, C-xy graphene conductivity value is of the same order as in pristine reduced GO (prGO), what in combination with its chemical reactivity make this FG perfect platform for bio- and gas sensing. Oppositely, C-ny graphene, containing up to 10 at.% of carbonyls, shows low conductivity and highly defective structure due to the formation of large number of 1-5 nm holes. As further shown, the introduction of new edge-located functional groups leads to significant changes in FGs work function and the valence band structure, namely appearance of new electronic states around 5-10 eV below Fermi level. Am graphene, the third studied FG with up to 7 at.% of amine groups attached to the graphene basal plane, exhibit C/O ratio of 11 and electrical conductivity of 290 $S*m^{-1}$ that is two-times higher than in prGO. The presence of amine groups is revealed to result in strong bending of graphene layers, leading to formation of mesoporous films and proved to allow the covalent bonding of various organic dyes and fullerenes to Am graphene. At the same time, the template synthesis has been determined to allow the synthesis of monodisperse CNDs 3.5 nm in size, consisting of ~7–10 defective functionalized graphene layers. Owing to their identical size and chemical composition, the CNDs found out to form primary aggregates ~30 nm in size via coagulation, which are, in turn, can form secondary porous spherical aggregates ~100 nm in diameter. The processes of coagulation of CNDs and peptization of their hierarchical aggregates are fully reversible and can be controlled by varying the MCND concentration or the pH value of the hydrosols. Further treatment of the obtained CNDs using wet-chemistry protocol has found to result in a seven-fold enhancement of their fluorescence efficiency, originating from the additional formation of new isolated sp^2 domains surrounded by defect sites [4].

[1] J. Phys. Chem. C 120, 28261 (2016)
[2] Scientific Reports 8, 14154 (2018)
[3] Nanoscale 10, 13223 (2018)
[4] Nanotechnology 30, 475601 (2019)

Charge distributions of iron photosensitizers probed with L-edge spectroscopies

R. Jay[1,2], S. Eckert[1,2], V. Vaz da Cruz[1], M. Fondell[2], P. Miedema[2], J. Norell[3], A. Pietzsch[2], W. Quevedo[2], J. Niskanen[2], K. Kunnus[4], R. Mitzner[2], A. Föhlisch[1,2]

1 Universität Potsdam, Germany
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
3 Stockholm University, Sweden
4 SLAC National Accelerator Laboratory, USA

Transition metal dyes based on earth-abundant elements like iron are promising systems for the design of inexpensive light-harvesting applications [1]. In order to optimize their performance with respect to the creation of long-lived electron-hole pairs, a fundamental understanding of both, ground and excited state electronic charge distributions is crucial. Here, we use X-ray absorption spectroscopy and resonant inelastic X-ray scattering at the iron L-edge whose selectivity to the relevant frontier orbitals grants direct access to the local valence electronic structure around the iron center. Thereby, the steady-state as well as transient charge distribution of the prototypical iron photosensitizer $[Fe(bpy)(CN)_4]^{2-}$ can be uniquely characterized.
The complex has been shown to exhibit a charge-transfer excited state with a picosecond lifetime [2], thereby being a suitable candidate for electron transfer processes. We show how the long lifetime can be correlated with effects in the metal-ligand covalency, where iron 3d electronic charge is delocalized onto the ligand [3]. The strong metal-ligand covalency observed for the ground state also plays a crucial role in the excited state, where it allows charge densities to be efficiently maintained locally at the iron center even after changes in the population of iron 3d orbitals. This is facilitated by an increase in electron donation from the ligand towards the metal due to a changed Coulomb-repulsion [4]. The associated electron-hole pair of the excited state can therefore not be correlated with significant changes in local charge densities, which challenges the common notion of charge-separation in transition metal dyes.

[1] Acc. Chem. Res. 49, 1477 (2016)
[2] Chem. Sci. 8, 515 (2017)
[3] Phys. Chem. Chem. Phys. 20, 27745 (2018)
[4] Angew. Chem. Int. Ed. 58, 10742 (2019)

X-ray absorption spectroscopy of the N_2^+ molecular cation

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

1 Lund University, Sweden
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
3 Uppsala University, Sweden
4 European XFEL GmbH, Germany
5 Technische Universität Berlin, Germany
6 Albert-Ludwigs-Universität Freiburg, Germany
7 IPCF-CNR, Italy
8 Henan University, P. R. China
9 KTH Royal Institute of Technology, Sweden

Investigation of X-ray absorption of molecular ions are important for advancement of fundamental molecular physics, especially for refinement of the description of highly excited states and challanging current theoretical models[1,2].

The X-ray absorption spectrum of the molecular ion N_2^+ has been measured using the Nano Cluster Trap end-station at beamline UE52-PGM at the BESSY II storage ring[3]. Ionic nitrogen was produced by leaking N_2 gas into an intense plasma created by He gas in a magnetron sputter source. The ions were directed via electrostatic fields and a radio frequency ion guide to a quadrupole mass filter where the N_2^+ was selected, and further guided to the ion trap. After X-ray absorption the excited molecules decay via Auger decay, leading to photofragmentation of the molecular cation. By recording the intensity of the photofragments as a function of the photon energy, ion yield spectra were obtained, which give a good representation of the X-ray absorption spectrum

The measurements allow for a detailed characterization of the first three ungerade core-ionized states excited from the $3\sigma_g^{-1}$ ground state of the ion by dipole transitions. The potential curves for these states are established via well-resolved vibrational progressions, and the lifetime width is measured. The observations are in excellent agreement with calculations from state-of-the-art quantum theory.

[1] J. Electron. Spectrosc. Relat. Phenom. 200, 78 (2015)
[2] J. Chem. Phys. 145, 224302 (2016)
[3] J. Phys. B: At. Mol. Opt. Phys. 42, 154029 (2009)

Poster Abstracts – Neutron Day at BER II

Wednesday, 4th of December

Twinning in $MAPbI_3$ - a case for the Laue diffractometer FALCON

Breternitz J, Tovar M, Schorr S

The physical properties of $MAPbI_3$, even its bare crystal structure, are still ground for debates and confusion. Concerning the latter, some confusion is due to typically heavy twinning that makes a reliable crystal structure determination complex. We studied these twinning effects and will second our experimental work by group-theoretical considerations to explain the possible effects occurring.

Elucidating the Internal Structure and Stability of Lubricating Films in Mammalian Joints

Dahint R, Schwörer F, Trapp M, Silvi L, Xu X, Dzubiella J, Steitz R

In our studies, we investigate the structure, molecular conformation and stability of thin phospholipid layers in contact with polyelectrolyte solutions. For DMPC coatings, we observed enhanced mechanical stability and a swelling behavior, which is strongly dependent on polyelectrolyte concentration. The experiments provide deeper insight in the mechanisms of wear reduction in mammalian joints.

Deuteration - curse or blessing: Chaos in the hybride perovskite $FAPbBr_3$

Franz A, Többens DM, Lehmann F, Kärgell M, Schorr S

We discuss the full structural solution of formamidinium lead tribromide and its temperature dependent phase transitions using neutron powder diffraction and synchrotron X-ray diffraction. Special emphasis is put on the influence of deuteration on formamidinium. It is shown that the deuteration critically influences the crystal structure of all three temperature modifications observed.

Order and disorder in a relaxor ferroelectric-thermoelectric oxide

Fritsch K, Nguyen H-H, Petsch A, Lu Z, Ye F, Hoffmann J-U , Yokaichiya F, Habicht K

We present a combined neutron scattering study of the temperature dependence of the crystal structure and the diffuse scattering in calcium barium niobate, a lead-free relaxor ferroelectric and proposed thermoelectric candidate oxide, using the instruments E2, FLEXX and CORELLI (SNS, ORNL).

Low energy phonons in a Tl-based chalcogenide thermoelectric material

Fritsch K, Ryll B, Lu Z, Winn B, Mamedov N, Habicht K

Understanding thermal transport at the microscopic level is imperative for the design of efficient thermoelectrics. Using FLEXX and HYSPEC (SNS, ORNL), we investigated the nature and temperature dependence of the low energy phonon modes proposed to be responsible for an intrinsically low lattice thermal conductivity in $TlInSe_2$, a ternary chalcogenide with quasi-one dimensional structural features.

Neutron waveguide for hydrogen detection in thin films

Guasco L, Khaydukov YN, Pütter S, Silvi L, Keller T, Keimer B

The impact of hydrogen into crystalline and amorphous solids is crucial both for fundamental science and technological applications. Neutron techniques have been used for many decades to study H in materials. In this poster we present a new method to measure small concentrations of H in thin films based on the dependence of resonance maximum in waveguide structures on the SLD of the middle layer.

The cold neutron triple-axis spectrometer FLEXX and its instrument options: MultiFLEXX and NRSE

Xu J, Lu Z, Hüsges Z, Meng S, Quintero-Castro DL, Toft-Petersen R, Groitl F, Habicht K

V2-FLEXX is a triple-axis spectrometer that offers a broad variety of operating modes. We highlight the capabilities of the multiplexing backend MultiFLEXX which provides the opportunity to do rapid overview measurements in wavevector-energy space and Neutron Resonance Spin-Echo spectroscopy which allows for linewidth measurements of excitations with an energy resolution in the μeV range.

Scientific highlights from the neutron triple-axis spectrometer FLEXX

Xu J, Lu Z, Hüsges Z, Meng S, Quintero-Castro DL, Toft-Petersen R, Groitl F, Habicht K

The high performance, flexibility and multiple options on the cold triple-axis spectrometer V2-FLEXX have continuously attracted interest from the international user community and made possible a significant number of high-impact research projects. Here we will show selected scientific highlights from our users exploiting the capabilities of FLEXX and its sample environment.

Structure-property relationship of Ba- and Ti co-doped $BiFeO_3$ ceramics

Karpinsky D, Silibin M, Latushka S, Zheludkevich D, Sikolenko V, Alikin D, Franz A

Concentration driven transition from rhombohedral to pseudocubic phase is accompanied by an increase in the unit cell volume and a decrease in tetragonality. Piezoelectric signal diminishes with the dopant content, while a switchable piezoresponse is observed for the compounds with pseudocubic structure; magnetization data show collinear antiferromagnetic state for the compounds with $x > 0.25$.

ESS Testbeamline V20 – Pilot Experiments for Future Neutron Source

Löhmann O, Kadletz PM, Woracek R

V20 is a dedicated instrument for tests of components and methods for the European Spallation Source. Here, we will present highlights of the work done in the last years. Results of imaging, reflectometry and SANS experiments and their data reduction processes will be explained. We will show that new concepts and methods will be able to handle both the high flux and high wavelength resolution.

Imaging of Water Distribution and Transport in Fuel Cells by Means of Neutron Imaging

Markötter H, Manke I, Arlt T, Kardjilov N, Kätzel J, Hilger A, Haußmann J, Klages M, Mohseninia A, Kartouzian D, Wippermann K, Schröder A, Sanders T, Banhart J

The water evolution and distribution in fuel cells are studied via neutron imaging. Visualizations and Quantifications of the water amounts in the membrane electrode assembly (MEA) as well as the gas diffusion layer and channel system via radiography and tomography are presented in this poster.

Polyelectrolyte Multilayer Films from Mixtures of Polyanions: Different Composition in Film and Preparation Solution

Sill A, Weltmeyer A, Nestler P, Paßvogel M, Neuber S, Helm CA

Films were made from PDADMA and binary mixtures of long PSSd and short PSS. With neutron reflectivity, it was found that the mole fraction of PSSd in the film was larger than in the deposition solution. On increase of adsorption time, long PSSd replaced short PSS. The studies show how to measure and control film composition when polydisperse polyelectrolyte solutions are used for film preparation.

Heat treatment induced residual stress relaxation in additively manufactured LPBF 316L stainless steel

Sprengel M, Ulbricht A, Evans A, Werner T, Kromm A, Bruno G, Kannengießer T

This investigation aims at elucidating whether heat treatments developed for conventionally manufactured stainless steel can be applied for Laser Powder Bed Fusion LPBF processed stainless steel, in order to relieve Residual Stress RS but maintain the benefits of LPBF specific microstructure. The triaxial bulk RS state was determined ex situ on the angle-dispersive E3 neutron diffractometer.

Magnetic frustration in $HoInCu_4$

Stockert O, Hoffmann J-U, Mühlbauer M, Senyshyn A, Koza MM, Tsirlin AA, Wolf FM, Bachus S, Gegenwart P, Movshovich R, Bobev S, Fritsch V

Little is known about magnetic frustration in metals. Combining powder and single-crystal neutron scattering and thermodynamic measurements allowed us to study the frustration in cubic $HoInCu_4$. Here holmium forms an fcc lattice giving rise to frustration and resulting in a partially disordered AF state and enhanced diffuse scattering. These findings are corroborated by thermodynamic measurements.

Noninvasive Imaging of Root-Soil Systems – Unveiling the Hidden Half

Tötzke C, Rudolph-Mohr N, Bereswill S, Kardjilov N, Oswald SE

How plants take up water and nutrients strongly depends on the transport properties of the soil close to the roots, a zone known as the rhizosphere. Combinations of neutron imaging with complementary X-ray or optical fluorescence imaging allow for detecting changes in structural and biochemical properties within the rhizosphere and provide a better understanding of root-soil interactions.

Neutron Laue diffraction at neutron source BER II

Tovar M, Allibon J, Raventos M, Budzianowski A, Rusinek D, Paliwoda D, Hoser A, Schorr S

The FALCON Laue diffractometer is designed for fast neutron Laue data acquisition applying wavelength band of 0.8-3.2 A. Examples for crystal orientation analysis as well as for 3D grain distribution mapping will be presented. Due to reactor stop there is on-going work to transfer the instrument to its new location at the Paul-Scherrer-Institute. Instrument re-commissioning is planned for 2020/21.

Understanding the cation distribution in $Zn_{1+x}GeN_2O_x$ ($x<0.1$) through neutron diffraction

Wang Z, Breternitz J, Franz A, Schorr S

Tuning the bandgap of absorber materials is critical for the development of high-efficiency solar cells. Zn group-IV nitrides as non-toxic, earth-abundant materials have attracted attention regarding a unique bandgap tuning mechanism depending on cation distribution or O incorporation. Herein, we use $Zn_{1+x}GeN_2O_x$ as an exemplary system to uncover cation distribution through neutron diffraction.

Poster Abstracts – Science Day at BESSY II

Thursday, 5th of December

2 Electronic structure and magnetic ordering in metal-free radical thin films

Junghoefer T, Baev I, Giangristomi E, Ovsyannikov R, Martins M, Calzolari A, Casu MB

We investigate thin films of an exceptionally chemically stable Blatter radical derivative by using X-ray based techniques. We observe X-ray magnetic circular dichroism at the nitrogen K-edge. Our results show magnetic ordering and calculations indicate, although weak, a long-range intermolecular coupling.

14 Spectroscopy Meets Chemical Vapor Deposition: Spatially Resolved Magnetic Field Effects on Thin Film Growth

Stadler D, Duchon T, Fischer T, Mueller DN, Mathur S

We report on the role of applied magnetic fields (0.5 T) during deposition of various oxides from alkoxides, leading to e.g. higher crystallinity and augmented out-of-plane magnetic anisotropy. X-PEEM in absorption mode helped us to demonstrate field-related effects with lateral resolution.

15 In aqua soft x-ray absorption spectroscopy of cerium oxide nanoparticles towards biomimetic applications

Duchon T, Xu S, Šmíd B, Fiala R, Arble CM, Kolmakov A, Cramm S, Schneider CM

Biomedical use of cerium oxide nanoparticles necessitates hydrophilic coating to avoid aggregation in human cellular environment. We directly access the surface electronic structure of the nanoparticles coated with polyacrylic acid and dextran in aqueous solution via a chip-based liquid-cell platform, providing insights into the role of the coating in enzyme mimetic activity.

16 Thermal phase design of ultrathin magnetic iron oxide films: From Fe_3O_4 to γ-Fe_2O_3 and FeO

Hamed MH, Duchon T, Mueller DN, Cramm S, Szyjka T, Müller M

Iron oxides have a wide range of applications, from catalysis to spintronics. In this work, we study the thermally induced redox reactions in ultrathin $Fe_xO_y/SrTiO_3$ heterostructures. The emerging phase transitions are driven by the thermodynamics of the interfaces. Precise identification and control of the phase transitions were achieved by step-wise annealing in the PEEM.

18 THz Electron Paramagnetic Resonance (EPR) for Molecular Nanomagnets, Life Sciences and Energy Materials Research

Lohmiller T, Nehrkorn J, Holldack K, Schnegg A

Spin couplings, often too large to be determined by conventional EPR, define functional properties and are sensitive to the structure of catalytic and magnetic molecules and materials. Frequency-domain THz-EPR at BESSY II enables mapping magnetic transitions over a wide energy/magnetic field range (3 to hundreds of cm^{-1} / <11 T). Here we present the upgraded experimental setup and recent results.

19 Controlled morphology and manganese doping of magnetosomes synthesized by bacterium Magnetospirillum gryphiswaldense

Marcano L, Gandarias L, Gandia D, Orue I, Valencia S, Abrudan R, Serrano A, García Prieto A, Muela A, Fdez-Gubieda ML

M. gryphiswaldense bacterium synthesize high quality cubo-octahedral magnetite nanoparticles with a mean diameter of 45 nm, called magnetosomes, suitable for numerous applications. In order to further expand their range of applications, the present work addresses the Mn doping of magnetosomes and provides experimental and theoretical findings concerning the role of Mn in their magnetic properties.

34 Absence of giant Rashba effect in the valence band of $CsPbBr_3$

Sajedi M, Marchenko D, Krivenkov M, Varykhalov A, Sánchez-Barriga J, Rader O

We have employed spin and angle resolved photoemission spectroscopy of $CsPbBr_3$ crystal to verify the presence of Rashba spin orbit coupling effect in the highest lying occupied state. We uncover the entire 3D BZ momentum space and the dispersion of the topmost bulk valence band at R point.

35 Graphene on Titanium Carbide: Intact Dirac Cones and Lifschitz Transition

Krivenkov M, Marchenko D, Golias E, Sajedi M, Sanchez-Barriga J, Frolov A, Fedorov A, Yashina LV, Rader O, Varykhalov A

We present first detailed report for the band structure of bare and graphene-covered TiC. We observe intact Dirac cones which are replicated according to the moiré nanopattern. Lifshitz transition leading to a strongly warped gear-shaped Fermi surface occurs, which is driven not by a mere doping effect of TiC by the graphene but by the unique interfacial hybridization in the band structure.

36 Photoemission studies of tetradymite-like natural heterostructures with magnetic and nonmagnetic atoms.

Frolov AS, Sánchez-Barriga J, Fedorov AV, Voroshnin VY, Tereshchenko OE, Sergeev AI, Yashina LV

Structural combining of topological insulators with trivial insulators is one of the ways to modify electronic structure and to bring a new properties such as ferroelectricity and magnetism. In present work, electronic and atomic structure of (111) surface of $(GeTe)(Bi_2Te_3)_2$ and $(MnTe)_{0.05}(Bi_2Te_3)$ topological insulators were probed by photoemission methods.

37 X-ray absorption spectroscopy at KMC-3 with cryogenic or in-situ sample conditions

Haumann M, Beyer P, Zaharieva I, Mebs S, Dau H

We operate an XAS station at beamline KMC-3 at BESSY II in cooperation with the HZB, dedicated to XAS in a ~3-13 keV range and open for user proposals. Recent progress includes a 13-element energy-resolving silicon-drift detector with rapid readout (≤1 ms) for time-resolved applications and in-beam electrochemistry. Experiments on (bio)chemical materials and future improvements are presented.

38 baSHELiXir: a tool for fast on-site experimental phasing

Kolenko P

Inaccessibility of exp. synchr. time on daily bases increases demand for fast evaluation of acquired experimental data. Such a requirement is crucial especially in the case of experimental phasing. The data quality can't be easily evaluated directly from data processing. For such case, a script baSHELiXir was designed. Novelty: space group search, parallelization. Support: SGS19/189/OHK4/3T/14

39 F2X Entry Screen – our new chemically diverse library with high hit rates

Wollenhaupt J, Barthel T, Metz A, Lima G, Wallacher D, Hauss T, Gerlach M, Feiler C, Wahl MC, Müller U, Klebe G, Weiss MS

Crystal structures of fragment-protein complexes provide starting points for structure-based compound development. Our new F2X Entry Screen of 96 compounds covers a large chemical space and performed excellently in our validation campaigns producing higher hit rates than previous libraries. In addition, the setup of the F2X Entry Screen in ready-to-use plates allows for experiments without DMSO.

40 Learning and teaching macromolecular crystallography: How to solve the phasing problem

Marbina S, Wollenhaupt J, Taberman H, Barthel T, Hauss T, Gerlach M, Weiss MS

Starting from previous macromolecular crystallography tutorials (Faust et al. 2008, 2010), four experiments were updated that solve the phasing problem in crystallography. Br-MAD, S-SAD, SIRAS and MR were performed on three well-known proteins, which provide meaningful diffraction data. The tutorial supply single step explanation from the raw data to structure determination for each experiment.

42 The HZB-MX BioLab

Gless C, Barthel T, Feiler C, Foerster R, Gerlach M, He H, Hellmig M, Kastner A, Lennartz F, Marbina S, Schnapka E, Steffien M, Taberman H, Weber G, Weiss MS, Wollenhaupt J, Hauß T

The HZB-MX BioLab supports the whole workflow from gene to crystal: cell cultivation, protein purification, crystallization and sample preparation. In addition, samples for other biological investigations, e.g. X-ray imaging and X-ray microscopy can be prepared. The BioLab is operated by the MX-group to support external and internal users for preparing their biological samples (safety level S1).

43 The Spectrolab for Macromolecular Crystallography

Hauß T, Gerlach M, Weiss MS

The HZB-MX-group Macromolecular Crystallography operates the SpectroLab next to the MX-beamlines. It is equipped with a micro-spectrophotometer which allows to measure the absorbance of tiny protein crystals in the UV-VIS spectral region. The microspectrophotmeter can be used off-line to detect changes in the absorption spectra in functional intermediates or due to e.g. radiation damage.

44 Facilities for Macromolecular Crystallography at the HZB

Gerlach M, Feiler C, Barthel T, Förster R, Gless C, Hauß T, He H, Hellmig M, Kastner A, Lennartz F, Marbina S, Schnapka E, Steffien M, Taberman H, Weber G, Wollenhaupt J, Weiss MS

The MX-group at the HZB operates 3 beamlines that are among the most productive MX-stations in Europe. They feature state-of-the-art experimental stations, serving 100 research groups across Europe. BL14.1 and BL14.2 are equipped with sample changer robots, providing a high degree of automation. At BL14.3 a new microdiffractometer, an HCLab device and a REX nozzle exchanger are available.

46 MXCuBE2 - Next-generation experiment control for macromolecular crystallography experiments at the BESSY II photon source

Hellmig M, Gerlach M, He H, Kastner A, Kornelsen O, Weiss MS

MXCuBE2 has been put into operation on all three HZB-MX beamlines. All beamlines share a unified user interface that integrates the interface to the automatic sample changer and the sample-centring functionality into the main control software. Furthermore it provides the basis for the implementation of new data-collection protocols as well as the integration of new instrumentation.

46a Novel type of sample holder as platform for macromolecular crystallography

Feiler CG, Wallacher D, Sarrou I, Mueller U, Weiss MS

Mounting a fragile protein crystal marks a decisive step in the workflow of X-ray crystallography. Novel types of patented sample holder overcome this issue. Apart from single-crystal diffraction, the holder serves as a fixed target in serial synchrotron experiment (SSX) approaches. Its minimal background scattering allows structure determination from weak data collected during an SSX experiment.

47 Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1

Faelber K, Dietrich L, Noel JK, Wollweber F, Pfitzner AK, Mühleip A, Sánchez R, Kudryashev M, Chiaruttini N, Lilie H, Schlegel J, Rosenbaum E, Hessenberger M, Matthaeus C, Kunz S, von der Malsburg A, Noé F, Roux A, van der Laan M, Kühlbrandt W, Daumke O

Mgm1 is a dynamin-like GTPase that is involved in membrane fusion and stabilization of cristae architecture. Since the molecular mechanisms were unknown, we solved the crystal structure and determined the assembly mechanism on membranes by cryo-ET. Whereas the domain composition of Mgm1 is similar to other dynamin superfamily members, the assembly model is remarkable different to that of dynamin.

48 Structural and functional principles of a novel family of nucleic acid helicases

Roske JJ, Liu S, Wahl MC

Nucleic acid-dependent NTPases are motor proteins that utilize NTP hydrolysis to remodel nucleic acids and nucleic acid-protein complexes or to unwind nucleic acid duplexes. We studied nucleic acid binding and unwinding activities of a helicase from a so far underexplored family in vitro and determined crystal structures of the enzyme in isolation and bound to a nucleic acid substrate.

49 Structure-Based Fragment Screening on Dynamin GTPase Domain

Taberman H, Daumke O, Weiss MS

Dynamin is a GTPase working in the endocytic pathway. It forms an oligomer around the neck of the invaginating vesicle, and the binding and hydrolysis of GTP introduce conformational changes inducing the membrane fission. Here, the HZB fragment screening workflow is used for finding novel small organic molecules occupying the binding site or allosteric sites for further drug development studies.

50 Tunable flexibility and porosity of the metal-organic framework DUT-49 through post-synthetic metal exchange

Bon V, Garai B, Krause S, Schwotzer F, Gerlach M, Senkovska I, Kaskel S

The post-synthetic metal exchange was used to afford DUT-49 frameworks with a wide variety of metal cations, eg. Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+} and Cd^{2+}. This approach is proven successful in achieving of rare examples of Mn-Mn and Cd-Cd dimers. Finally, heterometallic structures are formed by selective and controlled exchange of metal ions to finely tune the flexibility and NGA of the framework.

51 The structural basis for transmission blocking vaccines against malaria

Lennartz F, Brod F, Gologlu B, Mekhaiel D, Marini A, Sauerwein RW, Biswas S, Higgins MK

Developing a malaria vaccine that blocks parasite transmission from humans to mosquitos is a major priority in the fight against infectious diseases. Here, we structurally characterize inhibitory antibodies that bind Pfs4845, a key target for such a vaccine. With this, we design immunogens that display these epitopes, representing the first step towards the rational design of a new malaria vaccine

52 New beta-lactoglobulin variants with multiple binding sites for ligands

Loch J, Barciszewski J, Myszkowiak A, Pokrywka K, Jaskolski M, Lewinski K

Beta-lactoglobulin (BLG) is a small protein from lipocalin family. Crystal structures of selected new variants revealed that BLG can accommodate drug molecules not only in the primary binding site (beta-barrel) but also at the dimer interface. Determined structures indicated that engineered mutations can change not only binding specificity and selectivity but also stoichiometry of ligand binding.

53 Insulin polymorphism induced by p-coumaric acid: New crystal forms and advances in macromolecular powder diffraction

Triandafillidis DP, Parthenios N, Kosinas C, Spiliopoulou M, Valmas A, Gozzo F, Reinle-Schmitt M, Beckers D, Degen T, Pop M, Fitch A, Wollenhaupt J, Weiss MS, Karavassili F, Margiolaki I

This study focuses on the structural polymorphism of human insulin upon binding of the phenolic derivative p-coumaric acid over a certain pH range, through Powder and Single Crystal X-Ray Diffraction. Four polymorphs were identified, two of which were not reported previously. A novel structure of HI is also reported. The results of the study could be of great pharmacological interest.

54 Biochemical and structural characterization of an unusual cyanobacterial S-adenosyl-L-homocysteina hydrolase from synechocystis SP. PCC 6803

Czyrko J, Imiolczyk B, Sliwiak, J, Barciszewski J, Jaskolski M, Brzezinski K

SynSAHase in contrast to K^+-dependent SAHases, is not affected by the presence of any particular alkali ion. To explain this phenomenon, crystal structures of SynSAHase were determined for the enzyme crystallized in the presence of alkali cations. While SynSAHase shares common structural features with other SAHases, there is no alkali metal coordinated by the cyanobacterial enzyme.

55 Structural studies of mutants of the NaK channel

Minniberger S, Abdolvand S, Sun H, Plested A

Ionotropic glutamate receptors (iGluRs) mediate fast excitatory synaptic transmission in the central nervous system. Huge progress about functional mechanisms has been made but central questions concerning ion permeation and selectivity persist. Structures of mutants of the model channel NaK mimicking GluA2 give insights into the permeation mechanism, supported by molecular dynamics simulations.

57 Operando Soft X-ray Absorption Spectroscopy of the Solid Electrolyte Interface on Silicon Anodes in Lithium-ion Batteries

Schellenberger M, Hein D, Wartner G, Risse S, Seidel R

Silicon offers 11 times higher theoretical storage capacity than commercialized graphitic anodes. Currently, silicon anodes suffer from severe capacity fading, partly because the Solid Electrolyte Interface Layer fails to stabilize the electrolyte kinetically. We present an electrochemical cell for X-ray Absorption Spectroscopy to investigate the interface layer in operando during battery cycling.

58 SOL³PES – a new experimental setup for liquid phase soft X-ray photoemission spectroscopy at BESSY II

Hein D, Wartner G, Ali H, Pohl M, Winter B, Seidel R

We present the experimental setup SOL³PES equipped with a high-transmission hemispherical electron analyzer for soft X-ray photo- and Auger-electron spectroscopy from liquid phase that has been built for operation at BESSY II. Its name is derived from solid, solution, and solar, and refers to the aim of studying solid–liquid interfaces, optionally irradiated by photons in the solar spectrum.

59 Microstructured Si wafers for operando electrochemical IR spectroscopy

Lounasvuori M, Petit T

Microstructured silicon wafers with different groove angles are used as internal reflection elements in infrared spectroscopy. Bulk- and surface-sensitive measurements at different groove orientations are compared. The use of the wafers in operando electrochemical ATR-SEIRAS is demonstrated.

60 Irreversible Photoreactions stydied in-situ by a Time-Resolved Mid-Infrared Féry-Spectrometer at BESSY II

Ritter E, Puskar L, Hegemann P, Hofmann KP, Schade U

Sub-ms time-resolved IR spectroscopy has been limited to the study of cyclic systems where the same reaction can be repeated thousands of times. The Féry spectrometer at the IRIS beamline now overcomes this limit by exploiting the exclusive properties of infrared synchrotron radiation. Here we present this new, world-unique spectrometer together with first significant applications.

62 Design, fabrication and characterization of highly efficient multilayer blazed gratings for the tender X-ray region

Sokolov A, Huang Q, Senf F, Feng J, Lemke S, Alimov S, Knedel J, Kutz O, Seliger T, Gwalt G, Schäfers F, Siewert F, Sertsu M, Kozhevnikov IV, Qi R, Zhang Z, Li W, Wang Z

The optimization procedure of multilayer-coated blazed gratings (MLBG) design was systematically studied by numerical simulations. A test gratings with different blaze angles were fabricated and coated with the Cr/C multilayer. The MLBG with blaze angle of 1.0 degree showed a record efficiency reaching 60% at 3.1 keV and 4.1 keV.

63 Droplet Train for ambient pressure XPS at SpAnTeX

Clark P, Favaro M, van de Krol R, Starr D

We present an update on the new flow-focused droplet train module of the SpAnTeX endstation. This will enable stable XPS measurements on liquids in ambient coniditons for a range of applications. Advantages of the droplet train include a continuially refreshed sample (minimizing X-ray damage), and the Z-stability of droplets, allowing time-resolved measurements for e.g. nucleation and growth.

64 SpAnTeX: a new ambient pressure XPS endstation for exploring solid/liquid interfaces

Favaro M, Clark PCJ, Sear MJ, Drevon D, Johansson M, Maehl S, van de Krol R, Starr DE

SpAnTeX (SPectroscopic ANalysis with TEnder X-rays) is a new ambient pressure X-ray photoelectron spectroscopy (APXPS) endstation operating at the BESSY II synchrotron facility (at BL KMC-1 and UE56-2/PGM2). Here we show the commissioning performance of this new endstation, and highlight the experimental capabilities for in situ investigations of solid/gas, and solid/liquid electrified interfaces.

65 Elucidating the electrode-electrolyte interaction in high-temperature PEM-fuel cells by means of soft X-ray absorption spectroscopy

Wibowo EP, Garcia-Diez R, Felix R, Wilks R, Yang W, Prokop M, Bouzek K, Bär M

High-temperature proton exchange membrane fuel cells open new opportunities for intermediate temperature applications. A critical aspect influencing the cell's performance and durability is the interaction between the Pt catalyst on the electrode and the phosphoric acid electrolyte, which we aim to probe by using soft X-ray absorption spectroscopy at the phosphorus L-edge.

66 Tuning the porosity of IrO_2/TiO_2 catalysts: Towards Operando Monitoring of the Oxygen Evolution Reaction

van der Merwe M, Garcia-Diez R, Kasian O, Wilks R, Bär M

Titania-supported iridium oxide-based anodes are commonly used in water electrolysis. To perform operando O K-edge x-ray absorption and emission spectroscopy, enhancement of the porosity of IrO_x-based thin films is required to reduce the electrolyte signal contribution. Presented are new approaches to obtain mesoporous thin films of IrO_2/TiO_2 and first spectroscopic results on IrO_2/TiO_2 libraries.

67 Insights into the mechanochemical Knoevenagel condensation

Haferkamp S, Akhmetova I, Kulla H, Rademann K, Emmerling F

Mechanochemistry paves the way to simple, fast, and green syntheses, but there is a lack in understanding of the underlying mechanisms. Here, we present a universal strategy for simultaneous real-time in situ analysis, combining X-ray diffraction, Raman spectroscopy, and thermography.

68 A Comparative Study of Ionic Cocrystals

Linberg K, Ali N, Etter M, Michalchuk A, Rademann K, Emmerling F

The mechanochemical formation of the ionic cocrystals of glucose (Glc) and sodium salts is presented. Products are formed by co-milling Glc with three sodium salts (NaCl, NaBr, NaI). The reaction pathways of the three ionic cocrystals were investigated using our tandem approach comprising a combination of in situ synchrotron powder X-ray diffraction and Raman spectroscopy.

69 Synthesis of Bimetallic Nickel Nanoparticles for Catalysis

Bienert R, Prinz C, Emmerling F

We present the synthesis of monodisperse monometallic Ni nanoparticles (NPs) and bimetallic NiCu respectively NiCo NPs. The NPs were investigated using SAXS, STEM, EDX, and XANES, showing that the NPs are size tunable and stable. Nickel NPs have exhibited immense potential as important catalyst for the Sabatier reaction, i.e. converting waste to energy via transformation of CO_2 into CH_4.

70 Mechanochemical formation of transition metal phosphonates investigated in situ

Akhmetova I, Emmerling F, Roth C, Rademann K

Mechanochemistry is a versatile approach for green and fast synthesis of pure substances. The exploration of the chemistry of metal phosphonates has gained considerable interest during the last decades due to their structural divesity. We synthesized metal phosphonates in milling reactions. The mechanochemical reactions were investigated in situ to reveal the underlying mechanisms.

71 Multi-Scale Operando 4D Imaging and Machine Learning

Osenberg M, Hilger A, Sun F, Dong K, Schröder D, Wagner A, Binder J, Neumann M, Schmidt V, Birkholz O, Kamlah M, Janek J, Zahnow J, Klar P, Burkhardt S, Wetterauer S, Carraro T, Turek T, Banhart J, Manke I

We present 3D measurements on a wide range of materials. The propose is on the one hand a better understanding of manufacturing parameters and on the other hand the delivery of precise 3D multi class data sets for further material design and simulation.

72 Investigation of Rechargeable Zn-MnO_2 Batteries with X-Ray Tomography

Osenberg M, Dimitrova I, Hilger A, Kardjilov N, Arlt T, Markötter H, Manke I, Banhart J

We present in-operando X-ray tomographic investigations of the charge and discharge behaviour of rechargeable Zn-MnO_2 batteries. Changes in the three-dimensional structure of the zinc anode and the MnO_2 cathode material after several charge/discharge cycles were analysed. Results are compared to the behaviour of a conventional primary cell that was also charged and discharged several times.

73 In-operando synchrotron imaging of electrode materials in fuel cells

Markötter H, Haußmann J, Klages M, Seidenberger K, Wilhelm F, Arlt T, Scholta J, Manke I, Banhart J

The water distribution and evolution in a PEM fuel cell was studied via synchrotron imaging. The method development towards fuel cell research is presented in this poster. Water quantification and the identification of liquid water transport paths were conducted using radiography and tomography.

74 Local structure of SrF_2·EuF_3 luminescent nanoparticles: complementary XAFS and XRD study

Yusenko KV, Kabelitz A, Reinholz U, Radtke M, Krahl T, Guilherme Buzanich A

To yield an effective up-conversion of F-based matrices doped with rare earth elements, local structure was probed by XANES, EXAFS, XRD/PDF. We obtained hidden relations between composition, local structure, local environment and structural defects as well as light emission properties in unique class of novel luminescent materials with broad applications

74a Full field X-ray fluorescence imaging with coded apertures

Kulow A, Radtke M, Reinholz U, Buzanich A, Streli C

We developed a method for full field X-ray fluorescence imaging. An object is projected through a mask, producing overlapping images on the detector. To get the information about the object, a decoding step is necessary. We have developed and tested different decoding algorithms. First tests showed that a test object could be successfully reconstructed with our newly developed algorithm.

79 Tailor-made self-assembled monolayers with embedded dipole moments for interface engineering

Sauter E, Gärtner M, Nascimbeni G, Petritz A, Stadlober B, Zojer E, Terfort A, Zharnikov M

We present design and fabrication of particularly promising self-assembled monolayers (SAMs) utilizing the concept of embedded dipole. The experiments were combined with state-of-the-art band structure calculations. The SAMs allowed tuning the contact resistance of organic thin-film transistors over three orders of magnitude with excellent minimum values.

80 Triptycene tripods for the formation of highly uniform and densely packed self-assembled monolayers with controlled molecular orientation

Ishiwari F, Sauter E, Nascimbeni G, Tago H, Shoji Y, Fujii S, Kiguchi M, Tada T, Zojer E, Fukushima T, Zharnikov M

We present novel tripod systems for formation of well-defined self-assembled monolayers. These systems are based on the triptycene framework and enable strong binding to the substrate, large-area structural uniformity, precise alignment of functional groups, and control of their density. Consequently, they represent an ideal docking platform for complex and highly functional molecular films.

81 Surface Chemical Bond of Alternant vs. Non-Alternant Aromatic Isomers

Ruppenthal L, Klein BP, Herritsch J, Kachel SR, Hellweg L, Jaegermann AG, Heuplick LJ, Fan Q, Gottfried JM

Many organic semiconductors contain aromatic structures. We compare naphthalene as an alternant aromatic structure to azulene as its non-alternant isomer, on Cu(111) and Pt(111), using PES and NEXAFS. In addition, we compare the larger aromatic compounds pyrene and its isomer dicyclopenta[ef,kl]heptalene, as a model for the Stone-Wales defects in graphene.

82 Functionalized Nanographene Sheets as Efficient Inhibitors of Herpes Simplex Virus

Donskyi IS, Azab W, Cuellar-Camacho JL, Guday G, Lippitz A, Unger WES, Osterrieder K, Adeli M, Haag R

As resistance to traditional drugs emerges for treatment of virus infections, the need for new methods for virus inhibition increases. This study shows that antiviral agents against HSV-1 can be obtained by controlled and stepwise functionalization of graphene sheets and may be developed into antiviral agents for future biomedical applications.

102 Surfaces processes of perovskite-type electrode for SOFC studied in-situ by near-ambient pressure X-ray photoemission spectroscopy

Santaya M, Jiménez C, Carbonio EA, Garcia-Diez R, Arce M, Troiani H, Wilks R, Knop-Gericke A, Mogni L, Bär M

Ni-doped Sr(Ti,Fe)O_3 (STFN) perovskites are promising electrodes for solid oxide fuel cells. In reducing atmosphere, STFN ex-solves catalytically active Ni-Fe nanoparticles that improve carbon tolerance and lower operation temperatures. NAP-XPS in oxidizing and reducing atmospheres provides insights into the surface chemistry at the STFN/gas interface and reversibility of the ex-solution process.

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

Chen K, Luo C, Chen B B, Abrudan RM, Koster G, Mishra SK, Radu F

Charge transfer induced interfacial ferromagnetism and its impact on the exchange bias effect observed in the correlated oxide $La_{0.7}Sr_{0.3}MnO_3/NdNiO_3$ (LSMO/NNO) heterostructures is investigated by soft x-ray absorption (XAS) and x-ray magnetic circular dichroism (XMCD) spectra as a function of temperature, from 10 to 300K.

108 Observation of Compact Ferrimagnetic Skyrmions in $DyCo_3$ film

Chen K, Lott D, Philippi-Kobs A, Weigand M, Luo C, Radu F

We report the observation of compact ferrimagnetic skyrmions in $DyCo_3$ single layer, combining x-ray magnetic scattering, scanning transmission x-ray microscopy and Hall transport techniques. These skyrmions, with a characteristic lateral sizes of about 40 nm are formed during the nucleation and the annihilation of the magnetic maze-like domains with an obvious topological Hall effect character.

110 PEAXIS – The new soft RIXS spectrometer at BESSY II

Wong D, Schulz C, Bartkowiak M, Hofmann T, Habicht K

PEAXIS is a dedicated endstation that offers high resolution soft X-ray spectroscopy. We discuss RIXS spectra for a prototype perovskite ($SrTiO_3$) containing the electron-phonon coupling strength important for electron transport in quantum materials and $Ca_3Co_4O_9$, a misfit-layered thermoelectric oxide that probe the Co valence on crystallographic sites with different ligand environment.

111 In-Situ High Resolution X-Ray Microscopy To Image Crack Propagation In Microchips

Kutukova K, Liao Z, Werner S, Guttmann P, Standke Y, Gluch J, Schneider G, Zschech E

The full-field XRM at U41-PGM1-XM was combined with a special indenter manipulator to study fracture behavior of microchips. The experiments allow in-situ visualization of crack opening and propagation in Cu/low-k interconnect stacks. The study provides data regarding the robustness of BEoL stacks against thermomechanical stress and for the evaluation of the effectiveness of crack-stop structures.

112 X-ray microscopy in the tender X-ray range at the U41-PGM-XM beamline

Guttmann P, Werner S, Sokolov A, Siewert F, Huang Q, Senf F, Mast M, Rehbein S, Follath R, Schneider G

The X-ray microscopy beamline is designed for the photon energy range between 0.25 - 2.5 keV. The recently installed multi-layer grating and mirror in the plane grating monochromator allow now the access of the L-edges of transition metal oxides, as well as accessing the silicon, phosphor and sulphur K-edges to study crucial processes in cell membranes and catalysts. First results are presented.

114 Nanoscale NEXAFS as a tool for probing the doping of TiO_2 nanostructures: Nd, Eu and Ce

Bittencourt C, Acosta S, Ujiie T, Umek P, Werner S, Krüger P, Guttmann P

Due to the wide energy bandgap of TiO_2 doping is often used to optimize its use in a myriad of applications. We use Nanoscale NEXAFS to investigate the doping of isolated TiO_2 nanostructures with Eu, Nd and Ce. The susceptibility of the O K-edge and Ti L-edge to the local bonding environment in TiO_2-based materials makes NEXAFS ideal for providing both structural and chemical information.

114i ESUO - The European Synchrotron and FEL User Organisation

Arčon I, Arikan P, Bittencourt C, Boscherini F, Braz Fernandes FM, Brooks N, Casu B, D'Astuto M, Feiters M, Froideval A, Granroth S, Gross S, Gutt C, Hase T, Jablonska K, Jergel M, Kajander T, Khan A, Kirm M, Kokkinidis M, Kövér L, Lamba D, Larsen HB

The European Synchrotron and free-electron laser User Organisation (ESUO) established in 2010 is aiming at representing about 22.000 users. It is composed of 30 member countries. Our vision is to support a thriving (European) synchrotron and FEL user community with equal opportunities of access and participation for all scientists, based solely on the scientific merit of their ideas.

115 Probing electronic properties of metal-halide cations with soft X-ray absorption spectroscopy

Flach M, Gitzinger T, Zamudio-Bayer V, Kubin M, Bülow C, Timm M, von Issendorf B, Möller T, Lau T

Diatomic molecular transition-metal halides are simple model systems to study the effect of oxidation state, bond polarity, and electronegativity on L-edge excitation energy. We have used gas phase high-resolution XAS to study characteristic changes in L3-edge excitation energy and line shape of Iron and Nickel halides.

116 Probing the oxidation state of transition metal complexes: a case study on how charge and spin densities determine Mn L-edge X-ray absorption energies

Kubin M, Guo M, Kroll T, Löchel H, Källman E, Baker ML, Mitzner R, Gul S, Kern J, Föhlisch A, Erko A, Bergmann U, Yachandra V, Yano J, Lundberg M, Wernet P

The oxidation state of 3d transition metals can be sensitively probed with metal L-edge X-ray absorption spectroscopy, due to a characteristic shift of the L-edge absorption energy. In a combined experimental and ab-initio theoretical study we correlate this spectral shift, observed for high spin manganese complexes, with local charge and spin density differences at the manganese sites.

117 In situ PXRD during the gas adsorption on DUT-49-related MOFs involving ligands with variable elastic properties

Krause S, Bon V, Evans JD, Senkovska I, Többens DM, Wallacher D, Kaskel S

In situ PXRD during the physisorption of methane at 111 K and n-butane at 273 K shed a light on a structural contraction and reopening in a series of DUT-49 related materials, denoted as DUT-147, DUT-148, DUT-160, DUT-161 and DUT-162, showing a broad range of stiffness and as consequence – mechanical properties and Negative Gas Adsorption amount.

118 Zirconia-based thin films for energy applications

Mansilla Y, Arce M, Jimenez C, Basbus J, Gonzalez-Oliver C, Gamba N, Troiani H, Többens D, Serquis A

Zirconia-based materials are widely used for energy devices, such as electrolytes for Solid Oxide Fuel Cells. In this work, dense ZrO_2 and YSZ thin films were synthesized by sol-gel. These films were characterized by Grazing Incidence X-Ray Diffraction to determine crystalline features as a function of temperature. Results were contrasted with SEM, TEM, Raman Spectroscopy and conductivity tests.

119 MEAD and cation distribution in CZTSe, CFTS, and CZSiSe

Többens D, Gurieva G, Niedenzu S, Schuck G, Zizak I, Schorr S

Multiple Edge Anomalous Diffraction (MEAD) has been applied to $Cu_2ZnSnSe_4$, Cu_2FeSnS_4, and $Cu_2ZnSiSe_4$ semiconductors in order to validate the distribution of Cu^{+1}, Zn^{2+}, and Fe^{2+} in the crystal structure. Beamline KMC-2 has been upgraded to allow tracking the intensity of selected Bragg peaks over an absorption edge.

120 Investigating synergetic effects in SnO_x-modified CuO_x nanowire array CO_2 reduction electrocatalysts by hard and soft X-ray spectroscopy

Pardo-Perez LP, Stojkovikj S, Arndt A, Xi L, Mayer MT

Sub-nm ALD coatings of SnO_x grown onto CuO_x nanowire array electrodes cause drastic changes in catalyst selectivity, converting CO_2 to CO with selectivity >80% at low overpotentials. To unravel the origin of the synergetic effects of this mixed metal oxide system, we performed in situ hard XAS (bulk) and ex situ soft XAS (surface) characterization for the SnO_x-CuO_x electrocatalytic system.

121 First results of temperature-dependent EXAFS measurements with the Cryo-EXAFS environment at the multi-purpose beamline KMC-2

Schuck G, Többens DM, Wallacher D, Grimm N, Schorr S

The open concept of the KMC-2 beamline allows a wide range of sample environments. Here we present temperature-dependent Pb L3 edge EXAFS measurements of Cl-substituted $MAPbI_3$ measured at the newly build Cryo-EXAFS environment. The analysis of the EXAFS Debye-Waller factor of $MAPbI_3$ allows a direct determination of the influence of Cl substitution on the anharmonicity of the lead-halid bond.

122 XMCD of a molecular diamagnet: The peculiar case of Pd(II)

Schmitz-Antoniak C, Smekhova A, Schmitz D, Izarova NV, Stuckart M, Shams SF, Kögerler P

An intramolecular crossover from 2D diamagnetism to 3D paramagnetism has been found for Pd ions in polyoxopalladates. In the intermediate region, the large spin-orbit coupling facilitates a peculiar diamagnetic state modified by significant mixing, which exhibits a specific fine structure in both XANES and XMCD in an external magnetic field.

123 Sensitivity of 3d and 4f states to modifications of the local coordination symmetry

Schmitz-Antoniak C, Izarova NV, Stuckart M, Smekhova A, Schmitz D, Shams SF, Kögerler P

XANES, XMCD, and XMLD of polyoxopalladates hosting either 3d or 4f central ions revealed how changes to the local coordination symmetry modify electronic and magnetic properties. While the 3d states of Co(II) as well as the 4f states of Dy(III) and Ho(III) ions are highly sensitive to their local environment, the 4f states of Gd(III) remain largely unaffected.

124 Element-specific contributions to improved magnetic characteristics of Pd-decorated $CoFe_2O_4$ nanoparticles

Shams SF, Schmitz D, Smekhova A, Weschke E, Chen K, Luo C, Tavabi AH, Dunin-Borkowski RE, Radu F, Schmitz-Antoniak C

The total magnetic moments of 3d metal ions in bare $CoFe_2O_4$ and heterodimer Pd-$CoFe_2O_4$ nanoparticles probed by XAS and XMCD techniques show a significant increase after Pd decoration. In combination with a remarkable change in the field-dependent magnetization for Co ions this could be identified as a reason for improved heating performance in ac magnetic field.

126 Investigation of ultrafast optical manipulation of magnetic order in GdFe alloys and in an AFM/FM bilayer

Hosseinifar R, Kumberg I, Thakur S, Golias E, Fix M, Albrecht M, Kuch W

We study the stability of all-optical toggle switching in thin films of GdFe alloys after excitation with individual fs laser pulses using the SPEEM facility. The effect of coupling an antiferromagnetic (AF) film on the ultrafast demagnetization process of an adjacent ferromagnetic film is measured above and below the Néel temperature of the AF layer in pump-probe mode at the FemtoSpeX facility.

135 Core Lab Quantum Materials

Islam N, Feyerherm R, Klemke B, Siemensmeyer K

Methods offered by the quantum materials core lab are presented: - Synthesis and analysis of novel materials - Single crystal growth - Sample preparation: orientation, cutting, polishing, ... - Material characterisation using Squid and PPMS instuments: Magnetisation, specific heat, electric and thermal conductivity, ...

136 Neutron Diffraction Characterization on Momentive HOPG

Liu X, Qu H, Hasse U

Momentive's highly oriented pyrolytic graphite (HOPG) made by hot-pressed CVD pyrolytic graphite exhibits excellent mosaic spread for use as monochromator for neutron diffraction. Results on ZYA grade HOPG show 1.5x correlation between X-ray and neutron diffraction mosaic spread. This empirical correlation helps selecting HOPG grade. Momentive's HOPG shows good neutron reflectivity with optimal thickness ~1.2mm.

137 UNIFIT 2020 - the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

Hesse R, Denecke R

Main focus of the advancement of UNIFIT was the optimization of a dynamical memory management. The software offers the generation of animated gif files. After the export an animated gif file can be created with the software gifanimator.exe. The functionality of the right-mouse button for all different Unifit window types was improved according typical popup menus.

138 Relating Nanostructure to Macroscopic Properties Using A Laboratory Rheo-SAXS Setup

Ehmann HMA, Arlt B, Keilbach A, Pirolt F, Scheiflinger-Latal A

RheoSAXS gives you the unique chance to directly correlate structural changes with macroscopic properties. We present a novel experimental setup for performing combined RheoSAXS studies with the SAXSpoint 2.0 laboratory SAXS system.

140 Understanding texture formation in methylamine-recrystallised $MAPbI_3$

Smith JA, Game O, Martsinovich N, Shnier A, Kilbride R, O'Kane M, Flatken M, Wamwangi D, Parnell AJ, Billing D, Abate A, Lidzey DG

Methylammonium lead iodide can be crystallographically oriented, having enhanced carrier transport between interfaces, with various strategies to induce this texture. Here we use in situ GIWAXS using synchrotron radiation with 0.1 s time resolution to understand this evolution. We show intermediates form during the crystallization of the film, which exhibits complex non-uniaxial orientation.

146 New Scanning Transmission X-Ray Microscope (STXM) at the Energy Materials In-situ Lab (EMIL)

Weigand M, Wiesemann U, Wendt R, Raoux S

A new STXM for characterization of materials relevant for renewable energy technologies is under construction for placement at new branch of the EMIL soft X-ray beamline. Main design goal was flexible sample environment for operando measurement and vacuum sample transfer. The undulator beamline with high coherent flux will allow advanced imaging techniques and ps time resolved pump-probe imaging.

147 The EMIL Beamline(s) at BESSY-II: Status and Commissioning Results

Gorgoi M, Hendel S, Schäfers F, Gaupp A, Hävecker M, Frisch J, Lips K, Bahrdt J, Ries M, Raoux S, Viefhaus J, Bär M

The EMIL beamlines will provide high brilliance between 80 eV to 8 keV by employing two canted undulators, UE48 and U17. The soft x-ray branch is in friendly user operation while the hard x-ray branch is in commissioning using the full operating range of the U17 cryo-undulator. We will report on the energy resolution, photon flux, and focus size as well as on the commissioning progress.

148 Sputtertool at EMIL (Energy Materials In-situ Laboratory): Tailored thin film deposition for research at BESSY II

Steigert A, Novakovic N, Kronast F, Wartner G, Hein D, Silvi L, Raoux S

EMIL offers excellent infrastructure with various deposition methods (sputtering, evaporation, ALD, PECVD). Ultrathin multilayer systems such as Pt/CoFeB/Pt for laser driven formation of skyrmions were deposited, also materials for thermoelectrics (Al/SiGe and Au/SiGe). Depositions of thin films for research on materials for battery applications, coating of chips and ingots have been carried out.

149 Chemical & Electronic Surface Characterization of a Large NiO-Cu_2O Combinatorial Material Library by Photoelectron Spectroscopy

Bodenstein-Dresler L, Kama A, Hartmann C, Itzhak A, Hodes G, Wilks R, Cahen S, Bär M

A 72 x 72 mm^2 combinatorial library of NiO-Cu_2O, a promising HTL material for solar cells, was deposited by PLD and investigated by XPS to reveal composition-dependent chemical and electronic surface characteristics. These data are compared to complementary UV-vis and Air-PES data, to arrive at a complete picture of the material properties and allow first steps towards the tailoring of such.

153 Aqueous-phase Titanium Dioxide Nanoparticles: Nature of Water Adsorption and Structure of the Electric Double Layer

Ali H, Golnak R, Seidel R, Bergmann A, Meijer G, Xiao J, Winter B

We explore the mechanism of water dissociation at the anatase nanoparticle– aqueous solution interface, and characterize the electric double layer (EDL) that forms at this interface, by combining non-resonant (PES) and resonant (RPES) photoelectron spectroscopy, partial electron and partial fluorescence yield X-ray absorption spectroscopy (PEY-XAS, PFY-XAS) from an in-situ liquid microjet.

154 Probing the energetics of the MnO_4^{2-}(aq) transient ion using micro-mixing and liquid jet photoelectron spectroscopy

Mudryk K, Seidel R, Wilkinson I

We implemented a micro-mixing scheme to probe the electronic properties of a transient redox species – MnO_4^{2-}(aq) – using liquid jet photoelectron spectroscopy. We mapped the electronic structure of the aqueous ion and estimated its redox reorganization energy. The extracted energetics provide insight into the electrochemical behavior of the highly-reversible MnO_4^-(aq) / MnO_4^{2-}(aq) redox pair.

155 Metal-oxide electrode-electrolyte interfaces investigated by operando photoelectron spectroscopy

Hein D, Wartner G, Schellenberger M, Seidel R

We applied resonant (operando) XPS to reveal details of the OER mechanism of well-known catalytically active transition-metal oxides, e.g. Fe-Ni-OOH. We will present first experimental results from our (photo) electrochemical flow-cell, using graphene-covered Si_3N_4 and alkaline-ionomer based membranes as electron- and soft X-ray light-transparent interfaces.

156 High capacitance performance of multilayered $Ti_3C_2T_x$ MXenes driven by the Ti oxidation state probed via XAS

Al-Temimy A, Naguib M, Anasori B, Mazzio K, Golnak R, Lounasvuori M, Kronast F, Prenger K, Kurra N, Seredych M, Mawass M, Raoux S, Gogotsi Y, Petit T

MXenes is usually terminated by a mixture of –OH, –O–, and –F terminations but oxygen surface terminations are redox active. After cation intercalation, a dramatic enhancement in the electrochemical performance was observed. By applying the Ti L-edge sensitivity to probe the Ti oxidation state, this study shows that cation-intercalation alters MXene surface chemistry.

157 NEXAFS and XPS studies of the carbonized bath sponge scaffold and nanostructured 3D copper-carbon catalyst

Petrova O, Nekipelov S, Sivkov V, Molodtsov S, Ehrlich H

We examine the structural and chemical changes of bath sponge scaffold at temperatures at 1200 C in Ar and do the identification of copper phases at the surface of carbonized spongin scaffolds. Copper electroplating of the obtained composite leads to a hybrid material with excellent catalytic performance with respect to the reduction of p-nitrophenol in both freshwater and marine environments.

158 Reactivity of lithium with organic carbonates in ultra-high vacuum conditions

Rulev A, Frolov A, Itkis D, Yashina L

In our work we have studied reactivity of lithium towards propylene and ethylene carbonates in pure ultra-high vacuum conditions using XPS. The results have shown that the main products are lithium alkoxides, which differs from ones formed in liquid electrolytes. It may shed light on lithium chemistry, allowing to tune properties of SEI on lithium electrodes to address the whisker growth problem.

159 Hybrid h-BN-Graphene Monolayer with B-C Boundaries on a Lattice-Matched Surface

Bokai K, Tarasov A, Shevelev V, Vilkov O, Makarova A, Marchenko D, Petukhov A, Muntwiler M, Fedorov A, Voroshnin V, Yashina L, Laubschat C, Vyalikh D, Usachov D

Here, we report an approach to obtain a perfectly oriented and atomically thin hexagonal boron nitride-graphene heterolayer on the Co(0001) surface. High crystalline quality of the resulting interface allowed to uncover the structural and electronic properties of the lateral h-BN/Gr heterojunctions by means of complementary microscopic and spectroscopic techniques.

164 IRIS Beamline Microscopy Upgrade: Connecting Scales in Vibrational Imaging

Puskar L, Kneipp J, Schade U

A project to construct a new Synchrotron Microscopy Station for spatial- and polarization-resolved infrared spectroscopy at the IRIS beamline with the capability to record Raman spectra from the same sample spot has been approved by the BMBF funding. This collaborative project between Humboldt-Universität-Berlin and HZB will allow data acquisition across a broad range of lateral resolutions.

165 Reactive Metal-Organic Interfaces Studied with HAXPES: Modifying Reaction Depth and Interphase Formation

Kachel SR, Klein BP, Bock N, Krug CK, Ruppenthal L, Hochstraßer J, Fillsack F, Müller P, Schmid M, Gottfried JM

The vapor deposition of a metal onto an organic layer is followed by a diffusion of the metal atoms into the organic layer, where they react with the organic molecules, forming an interphase. Here, we studied two different systems, Ca on 6T and Co on 2HTPP with HAXPES. We varied process parameters such as sample temperature during interphase preparation and investigated the reaction depth.

166 Annealing of $Cu(In,Ga)Se_2$ absorbers with CdS and Zn(O,S) buffers - an in situ hard X-ray photoelectron spectroscopy study

Wenisch R, Kodalle T, Maticiuc N, Wang Y , Bertram T, Hasan AY, Deumer J, Knoop S, Kaufmann CA, Schlatmann R, Lauermann I

This study employs in-situ, hard X-ray photoelectron spectroscopy to investigate the thermal degradation mechanisms of the $CuInGaSe_2$/buffer interface are investigated. Both CdS and Zn(O,S) buffer-layers and RbF post-deposition treatment are examined. The temperature was ramped up from 150°C to 350°C at 0.5°C/min, resulting in a quasi-continuous temperature resolution.

167 Thermally Induced Chemical Interactions Across Emitter/$Cu(In,Ga)Se_2$ Thin-Film Solar Cell Interfaces Probed by Photoelectron Spectroscopy

Valenta D, Yetkin HA, Kodalle T, Bombsch J, Garcia-Diez R, Hartmann C, Wilks RG, Kaufmann C, Bär M

Thermal input can trigger chemical interaction processes across interfaces in $Cu(In,Ga)Se_2$–based thin-film solar cell layer stacks. While Na diffusion into the absorber is beneficial, the diffusion into the emitter region deteriorates cell efficiency. We use photoelectron spectroscopy to study annealing-induced changes at different buffer/$Cu(In,Ga)Se_2$ interfaces with a focus on Na diffusion.

168 Sodium intercalation in TiO_2 electrodes during dis/charging of sodium ion batteries monitored by operando XANES measurements

Siebert A, Dou X, Félix R, Klemke B, Greco G, Hasa I, Handick E, Wilks RG, Garcia-Diez R, Passerini S, Bär M

We report an operando Ti K-edge absorption study which monitors the insertion of Na into anatase TiO_2 nanoparticle-based anodes by probing through the charge collector while dis/charging the battery. Amorphisation of the anatase structure and changes in the number of nearest neighbors of the Ti atom and the Ti oxidation state (from Ti^{+4} towards Ti^{+3}) during (de)sodiation were observed.

169 In situ Characterization of Lithium Deposition at Lithium Anode by Synchrotron X-ray Tomography

Dong K, Osenberg M, Markötter H, Sun F, Manke I, Hilger A, Arlt T, Banhart J

Li deposition at the Li/separator interregion was visualized under in situ condition. The deposition within Celgard 2325 separator has been firstly characterized in 3D. In addition, a porous carbon fiber matrix was selected for analysing and quantifying Li deposition within this matrix in 3D and unravelling the deposition behavior.

170 Multiscale imaging for alkaline water electrolysers

Arlt T, Evangelisti C, Markötter H, Liebert M, Paulisch M, Röntzsch L, Rauscher T, Mohseninia A, Bergbreiter C, Kaczerowski J, Jörissen L, Manke I

Electrolyzers are a key factor for the energy transition from fossil to renewable energy as they are versatile converters with a wide area of application. Media transport processes are still a crucial point. Especially the sintering process of transport layers is critical since the homogeneity strongly impacts the cell performance. Multiscale imaging methods deliver valuable results.

171 Accessing carbon inks on ancient papyri using synchrotron radiation

Mahnke H-E, Arlt T, Schade U, Siopi T, Manke I, Lepper V

A multitude of papyri is stored in the Papyrus Collection of the Egyptian Museum Berlin. To get access to this source of knowledge about our cultural origin we have to reveal hidden texts. While it is feasible to detect metal-containing inks by hard X-rays, i.e. absorption and absorption edge tomography, carbon inks are more difficult to detect. THz imaging turned out to be a possible complement.

172b Evolution of porosity, crack density, and CMAS penetration in thermal barrier coatings

Müller BR, Mack DE , Laquai R, Helle O, Sebold D, Vaßen R, Bruno G

Degradation of thermal barrier coatings (TBCs) in gas-turbine engines due to calcium-magnesium–aluminosilicate (CMAS) glassy deposits has been study by Synchrotron Refraction Radiographie and state of the art electron microscopy to elucidate the intrusion of CMAS into the porous structure of atmospheric plasma sprayed TBCs and the formation and growth of cracks under thermal cycling.

172c Investigation to elucidate Vanadium crossover in novel membranes for Vanadium Redox Flow Batteries

Lutz C, Hampel S, Ke X, Beuermann S, Kunz U, Turek T, Guilherme Buzanich A, Radtke M, Fittschen UEA

VRFB are currently one of the most promising candidate for stationary chemical energy storage. For large scale applications the ion conducting membranes currently in use need to be improved. Here we present the evaluation and comparison of the XANES spectra of the vanadium species in Nafion 117 and in novel membranes and that reactions could take place inside the membranes nanosopic water body.

173 Surface refinement of biodegradable polymer PBAT with thin a-C:H layers

Schlebrowski T, Nefedov A, Wehner S, Fischer CB

The poor degradability of many polymers leads to a major waste problem. A solution are polymers that are biodegradable like polybutylene adipate terephthalate (PBAT). In order to adapt it to the desired applications, it can be coated with amorphous hydrogenated carbon layers (a-C:H). Here we present a detailed analysis of the a-C:H coated surface with different film thicknesses on PBAT.

174 Switching of laterally mounted Azobenzene on platforms adsorbed on Au(111): A Surface-Spectroscopy Study

Schlimm A, Strunskus T, Lautenschläger I, Rusch T, Hammerich M, Herges R, Magnussen O, Tuczek F

Rotors and switches are elementary building blocks of molecular machines. While vertically oriented switches and rotors have been obtained by various strategies, we here demonstrate a molecular adlayer system with laterally oriented azobenzene that combines photoswitching and rotation. The molecules form well-ordered monolayers on Au(111) with the azobenzene units parallel to and above the surface.

175 Angle dependent deposition of a-C:H layers on biopolymer polylactide acid (PLA) - A chemical composition examination

Beucher L, Schlebrowski T, Fritz M, Fischer CB

Polylactide acid (PLA) is a biodegradable polymer used in industrial applications. For some applications it is necessary to change they surface properties. These can be modified with thin amorphous hydrogenated carbon (a-C:H) coatings produced by plasma enhanced chemical vapor deposition (PECVD). Their sp^2 and sp^3 content is directly dependent on the deposition angle between sample and plasma.

176 Investigation of molecular orientation and interfaces by means of NEXAFS spectroscopy

Bischof D, Kothe M, Breuer T, Witte G

NEXAFS spectroscopy is a versatile tool for the analysis of the molecular orientation and the identification of molecules. An example is the molecular orientation of a phthalocyanine semiconductor, which is strongly influenced by the substrate quality. The second example is the interface between acenes and fullerenes, where the temperature-induced formation of Diels-Alder adducts is revealed.

177 Surface Reactions on Molybdenum Disulfide Catalysts

Kuznetsov V, Fouquet P, Traeger F, Jagodar A, Kovacevic E, Strunskus T, Nefedov A, Wöll C

There is a growing interest in alternative catalysts as cost efficient substitutes for noble metals for electrochemical applications including water electrolysis. On electrodes loaded with MoS_2 and also on single crystal reference materials, several reactions of the surfaces are found using X-ray photoelectron spectroscopy (XPS). Results on hydrogen diffusion will be related to surface chemistry.

178 NEXAFS analysis of carbon nanowall composites

Jagodar A, von Wahl E, Berndt J, Strunskus T, Cvelbar U, Boulmer-Leborgne C, Kovacevic E

In this work the synthesis (plasma) and analysis of CNWs and graphene nanocomposites will be presented. The material structure, e.g. morphological, chemical and microstructural features, is revealed by employing near edge X-ray absorption fine structure (NEXAFS) spectroscopy, in combination with X-ray photoelectron spectroscopy (XPS), on the HE-SGM beamline.

179 Orthogonal Switching of Two Rotaxanes Assembled in Multilayers on Surface

Hupatz H, Heinrich T, Wagner A, Unger WES, Schalley CA

Herein, we present mixed multilayers where two different rotaxanes were deposited in separate layers. For the first time, we show successful orthogonal on-surface switching induced by chloride ions and light. We used NEXAFS spectroscopy and SR-XP spectroscopy to study structural effects in multilayers and reversibility upon switching.

194 X-ray Magnetic Circular Dichroism Study Cu-BDC SURMOF-2 structures

Nefedov A, Müller K, Radu F, Golias E, Heinke L, Kuch W, Wöll C

Metal-organic frameworks (MOFs) are crystalline self-assembled solids from metal compounds and organic ligands. Recently, it was reported on the ferromagnetic ordering in SURMOF-2 series of CuBDC MOFs with a Curie temperature above 20 K. Here we present results of XMCD study both pristine CuBDC SURMOF-2 structures and after their loading with metallocenes.

195 Temperature-, light-, and x-ray-induced spin crossover of molecules adsorbed on a graphite surface

Torres J, Kipgen L, Kumberg I, Ossinger S, Thakur S, Arruda L, Hosseinifar R, Golias E, Tuczek F, Kuch W

The spin-state transition of 0.4 molecular monolayers of the complex $Fe(H_2B(pz)(pypz)_2$—which is in the low-spin (LS) state at temperatures up to RT in bulk— on graphite is probed at low temperatures by XAS. At 10 K, it undergoes both a light- and an x-ray-induced transition to the high-spin state; on raising the temperature to 120 K, it reverts back to the LS state, showing spin-state reversibility.

196 X-ray magnetic linear dichroism as a probe for non-collinear magnetic state

Luo C, Ryll H, Back C, Radu F

We report on exploiting XMLD contrast for probing the non-collinear states in DyCo and FeGd ferrimagnetic thin films. An anomalous 'wing shape' hysteresis loop is observed slightly above its compensation temperature due to the formation of an the out-of-plane domain wall formation from the surface towards the bulk, which is directly observed via XMLD measurements.

197 High-resolution X-ray Spectroscopy - Experiments and Theory

Bzheumikhova K, Hönicke P, Wansleben M, Kayser Y, Unterumsberger R, Holfelder I, Zech C, Vinson J, Jach T, Beckhoff B

The electronic structure of matter is explored using X-ray absorption spectroscopy (XAS) , X-ray emission spectroscopy (XES), and resonant inelastic X-ray scattering (RIXS), which is in it's simple description a combination of XAS and XES. The experimental results are compared to calculations of core-level spectroscopy based on ground-state (DFT) calculations and the Bethe-Salpeter equation.

198 A Compact Vibration Compensating Setup for Scanning nm-XRF and STXM

Wählisch A, Seim C, Lubeck J, Unterumsberger R, Hönicke P, Kayser Y, Hoehl A, Fleischmann C, Rehbein S, Dehlinger A, Haidl A, Weimann T, Dai G, Beckhoff B

We present a novel instrumentation for synchrotron radiation based scanning XRS, where all relevant optical elements are mounted on a single platform. This compact setup minimizes vibrations, enabling a spatial resolution in the nm regime with STXM and scanning XRF analysis. We demonstrate a reference-free quantification method based on XRF on a nanostructured germanium sample.

199 Reference-free quantification of microliter-droplets using Total Reflection and Grazing Incidence X-Ray Fluorescence analysis

Unterumsberger R, Gross A, Stosnach H, Hönicke P, Beckhoff B

Reference droplets for TXRF analysis have been investigated with respect to the lateral spreading and absolute mass deposition. The lateral spreading can affect the effective solid angle of detection and influence the X-ray Standing Wave field due to shadowing effects for small incident angles. The results show the importance of well-characterized reference samples for TXRF applications.

200 Extracting Dimensional Parameters of Gratings Produced with Self-Aligned Multiple Patterning Using GISAXS

Pflüger M, Kline RJ, Fernández Herrero A, Hammerschmidt M, Soltwisch V, Krumrey M

New approaches are needed for the fast, non-destructive measurement of nanostructures, e.g. in the semiconductor industry. GISAXS has the potential to fulfill these needs, but the analysis of the data is complicated. We reconstruct line shape, pitch error, and their uncertainties from GISAXS measurements of a series of 32 nm grating samples produced by self-aligned quadruple patterning.

200a Analysis of vibration-based degradation of the spatial resolution of a nanometer-X-ray fluorescence analysis setup

Peinl F, Holfelder I, Lubeck J, Weser J, Beckhoff B

The work involves a frequency and amplitude-dependent analysis of the impact of the vibrations on the spatial resolution of the nm-XRF setup of the PTB. Two kinds of additional complementary experiments were performed: two different nm-XRF instruments were characterized at the same site of the PGM beamline and one of the nm-XRF instruments was characterized at the PETRA III P04 beamline.

200b Determination of Optical Constants in the EUV Spectral Range

Saadeh Q, Soltwisch V, Naujok P, Scholze F.

In the EUV spectral range the optical parameters of many materials are not well known or based on calculations. The aim here is to reconstruct the optical parameters of materials from the reflectivity measurements of stratified systems. In this study, we will present the feasibility of determining the optical constants for candidate materials for EUV Photomask Absorbers using EUV reflectometry.

200c Studying gases and volatile organic compounds by using TXRF and XAS in an in situ gas cell

Streeck C, Grötzsch D, Weser J, Malzer W, Mantouvalou I, Kanngießer B, Beckhoff B

The in situ measuring cell is designed especially for applications in the soft X-ray range. Thus, elements of interest like C, N, and O can be measured in transmission and their X-ray fluorescence signal. Furthermore also the sorption behavior on surfaces can be studied under total X-ray reflection geometry. The results of the XAS studies on Ethanol at the C and O K-edge are shown.

CR1 Magnetization switching via individual femtosecond laser pulses in a $DyCo_5$ thin film grown on a nanofacetted GaAs substrate

Luo C, Erb D, Chen K, Marcano L, Mawass MA, Molina SV, Kronast F, Abrudan R, Radu F

We present a study of all-optical switching by single femtosecond laser pulses on a ferrimagnetic $DyCo_5$ thin film. Utilizing X-PEEM technique we observe magnetization switching for different laser fluences which exhibit a threshold character in absence of magnetic field. This type of magnetic switching occurs at different ambient temperatures above and below the compensation temperature.

CR2 Skyrmion nucleation and manipulation by ultrafast laser pulses

Novakovic N, Mawass MA, Steigert A, Engel D, Kronast F

Writing and erasing skyrmions by local heating through a laser has been predicted theoretically. Here, we analyze these processes as a function of circularly polarized laser pulses. We investigate the possibility of deterministic formation and annihilation of skyrmions in different ferro- and ferrimagnetic systems. PEEM was used for magnetic imaging.

CR3 Effect of confinement on chemical reactions: water formation under a silica bilayer

Prieto M, Mullan T, Schlutow M, Gottlob D, Tanase L, Menzel D, Sauer J, Usvyat D, Schmidt T, Freund H-J

We show results obtained with the SMART microscope, using in situ XPS, LEED and LEEM. Silica thin films supported on Ru(0001) are used as a model system to study how physical confinement can affect the kinetics of the water formation reaction. A combined approach of experiments with DFT simulations and kinetic modelling allow us to identify which elementary steps are affected.

CR4 Spectromicroscopic Investigation of Plasma Activated Copper for Carbon Dioxide Electroreduction Reaction

Tanase LC, Prieto MJ, de Caldas Souza L, Grosse P, Scholten F, Schmidt T, Roldan Cuenya B

Cu oxidation using a plasma source and CO_2 electroreduction reaction have been studied by combining LEEM, LEED, NEXAFS, XPEEM and XPS in order to resolve local inhomogeneities in the morphology, crystallinity and chemical state of the surface. Different oxidation and local properties are identified based on the crystal orientation and on the type of the EC treatment.

PTB1 Towards operando EXAFS investigations of advanced piezoelectric materials

Kayser Y, Hönicke P, Wählisch A, Cain M, Thompson P, Beckhoff B

Within the EMPIR project ADVENT, EXAFS is applied to record the response of PZT-films to alternating electric fields applied at a frequency in the megahertz range. The current progress towards time-resolved traceable atomic coordination measurements of piezoelectric materials proposed for the next generation of ultra-low power energy-efficient devices will be presented.

PTB2 Limits of application of the Debye-Waller factor for the determination of roughness in GISAXS

Fernández Herrero A, Pflüger M, Probst J, Scholze F, Soltwisch V

The effect of line edge roughness of lamellar gratings on the diffracted intensities has been systematically analysed with a dedicated set of samples. For the description of the impact of the roughness, a Debye-Waller factor (DWF) is usually used. We investigate to which extent the DWF is applicable for the description of the impact of the line roughness on the scattering pattern from GISAXS.

PTB3 Using grazing incidence X-ray fluorescence for characterization and element sensitive reconstruction of nanostructures

Andrle A, Hönicke P, Schneider P, Kayser Y, Hammerschmidt M, Burger S, Scholze F, Beckhoff B, Soltwisch V

A method based on GIXRF measurements is applied to Si_3N_4 lamella gratings. This technique is based on the XSW field effect and is sensitive for the elemental composition and geometric shape of the nanostructures. With a finite element Maxwell solver, the XSW field can be calculated and used to model experimental data and thus derive the spatial element distribution and the geometric shape.

PTB4 Photon Detector Calibration in the EUV spectral range at PTB

Laubis C, Babalik A, Babuschkin A, Barboutis A, Buchholz C, Fischer A, Jaroslawzew S, Lehnert J, Mentzel H, Puls J, Schönstedt A, Sintschuk M, Stadelhoff C, Tagbo C, Scholze F

Detectors range from diodes to CCDs. Lifetime and homogeneity requirements are common among detector uses with sensitivity targets from single photon to reduced sensitivity for dose control. PTB employs EUV beamlines for radiometric characterizations of photon detectors. The wavelength range reaches from 1 nm to 45 nm. Lifetime testing at PTB's exposure setup offers power densities up to 20 W/cm^2.

PTB5 How Metrology Can Improve Photoemission Tomography

Kirschner H, Gottwald A, Richter M, Koller G, Ramsey M, Puschnig P, Soubach S, Tautz S

Photoemission tomography (PT) is a proven tool to measure the electron distribution of oriented molecular layers on surfaces by angle-resolved photoemission spectroscopy. We seek to generalize PT by applying it to gas-phase atomic photoelectron emission data with regard to a possible reconstruction of atomic orbitals, thus opening a path for absolute quantification.

PTB6 Effective and calibratable wavelength-dispersive high-resolution X-ray emission spectrometer for polarization-dependent measurements in the soft x-ray range

Holfelder I , Kayser Y, Müller M, Peinl F, Unterumsberger R, Stadelhoff C, Weser J, Beckhoff B

For a better understanding of the electronic structure of 2-D systems, a new wavelength-dispersive spectrometer (WDS) is developed at the PTB in cooperation with NIST. To increase the solid angle of detection spherical mirrors and variable line spacing (VLS) gratings in two detection arms (one perpendicular to the storage ring plane) are used. We present the concept and design of the spectrometer.

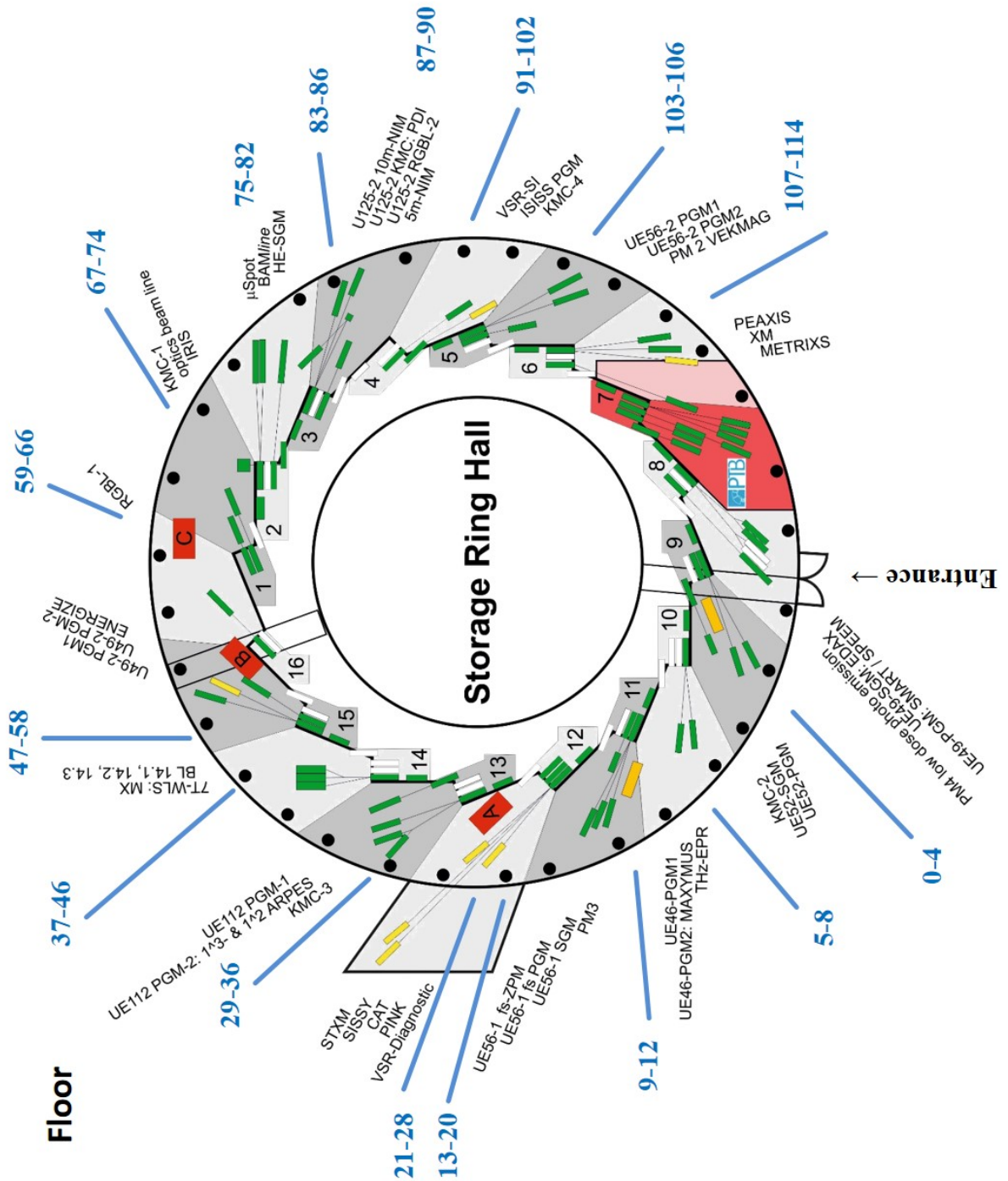
PTB7 VUVR: an optimized Beamline for VUV-Radiometry

Ogor O, Fliegauf R, Hain S, Kaser H, Kroth U, Gottwald A

A new VUV-Beamline with a 2m normal-incidence off-plane eagle type monochromator will substitute the old 1m NIM-Beamline at the Metrology Light Source. Its design aims for higher flux, better optical image in and out of focus, higher level of automation and the opportunity of multiple experimental stands. Higher wavelength-resolution is not a primary goal but will also be achieved.

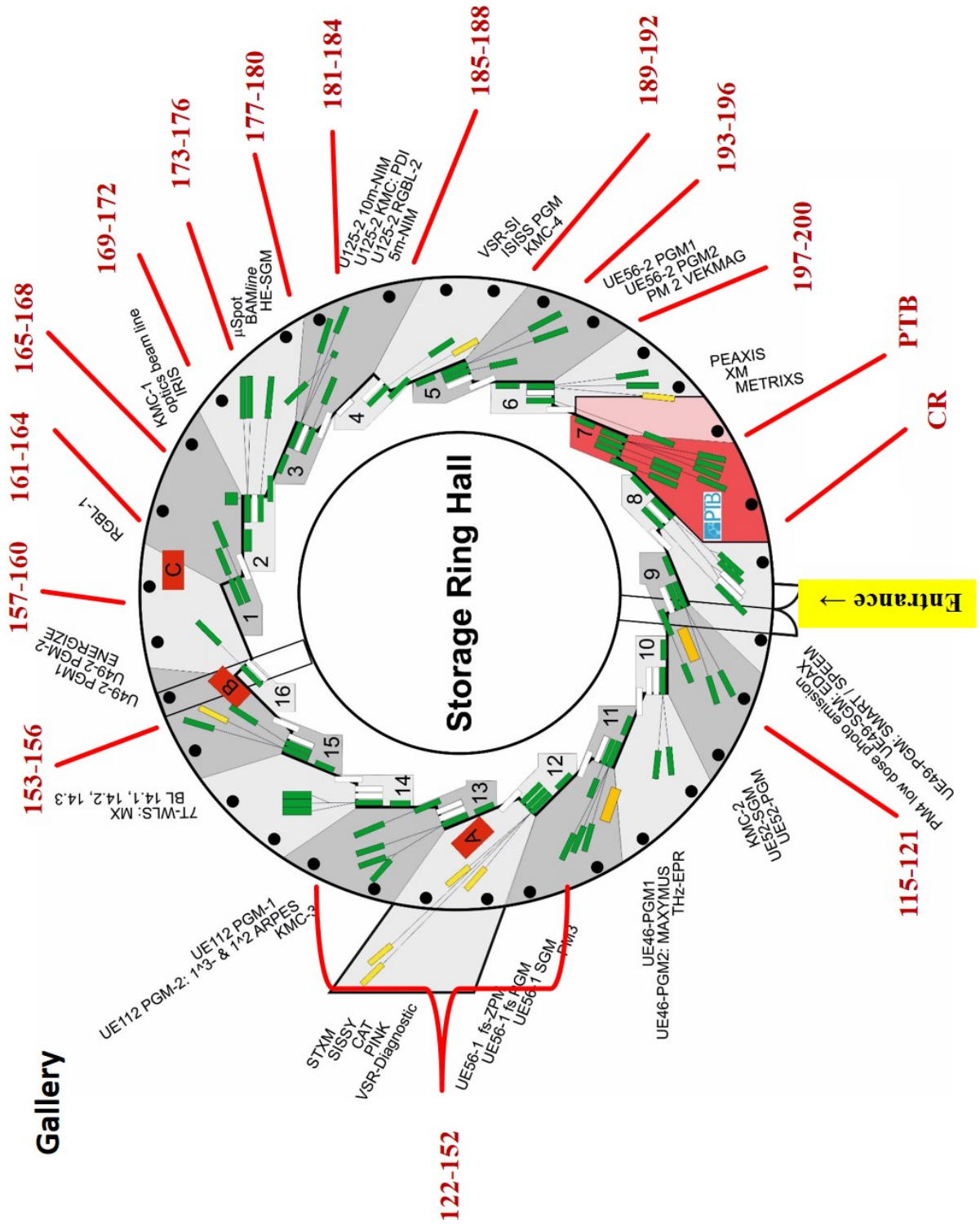
Floor Plan Poster Session – Science Day at BESSY II

Thursday, 5th of December



Floor Plan Poster Session – Science Day at BESSY II

Thursday, 5th of December



Vendor Exhibition

Vendor Logos

Vendor Addresses

Agilent Technologies
Lyoner Str. 20
60528 Frankfurt/M., Germany
www.agilent.com
johannes.schuricht@agilent.com

Alca Technology Srl
Via Lago di garda 130
SCHIO (VI), ITALY
+393496096784
www.alcatechnology.com
andrea.lanaro@alcatechnology.com

Allectra GmbH
Traubeneichenstr. 66
16567 Schoenfliess, Germany
+491783373104
www.allectra.com
b.holmes@allectra.de

attocube systems AG
Eglfinger Weg 2
85540 Haar, Germany
www.attocube.com
patrizia.kellner@attocube.com

AXON' Kabel GmbH
Hertichstr. 43
71229 Leonberg, Germany
+4971529799283
www.axon-cable.com
m.stuible@axon-cable.de

BESTEC GmbH
Am Studio 2b
12489 Berlin, Germany
+493067099211
www.bestec.de
sabine.proll@bestec.de

Carl Zeiss SMT GmbH
Rudolf-Eber-Strasse 2
73447 Oberkochen, Germany
+497364205971
https://www.zeiss.com/smt
norman.niewrzella@zeiss.com

Cryoandmore Budzylek GbR
Hermann-Cossmann-Str. 19
41472 Neuss, Germany
+4952154362710
www.cryoandmore.de
christian@cryoandmore.de

FMB Feinwerk- und Messtechnik GmbH
Friedrich-Wöhler-Str. 2
12489 Berlin, Germany
+493067773057
www.fmb-berlin.de
j.jaehnigen@fmb-berlin.de

FOCUS GmbH
Neukirchner Strasse 2
65510 Huenstetten, Germany
+496126401431
https://www.focus-gmbh.com
d.pohlenz@focus-gmbh.com

FuG Elektronik GmbH
Am Eschengrund 11
83135 Schechen, Germany
+4980394007780
https://www.fug-elektronik.de/
schmoeller.h@fug-elektronik.de

Goodfellow GmbH
Alsterwiete 3
20099 Hamburg, Germany
+49800100579
Goodfellow.com
Karin.Hildyard@goodfellow.com

greateyes GmbH
Justus-von-Liebig-Str. 2
12489 Berlin, Germany
www.greateyes.de
axel.wiegand@greateyes.de

Hiden Analytical Europe GmbH
Kaiserswerther Strasse 215
40474 Düsseldorf, Germany
+447775445759
www.hideneurope.de
luke.wells@hideneurope.de

Hitachi High Technologies Science America Ltd.
20770 Nordhoff St
Chatsworth CA 91311, USA
+12144370368
www.hitachi-hightech.com/hhs-us/products/index.html
del.redfern@hitachi-hta.com

Hositrad Vacuum Technology
De Wel 44
3871 MV Hoevelaken, Netherlands
+31332537210
+491605627540
www.hositrad.com
andre@hositrad.nl
info@hositrad.com

Huber Diffraktionstechnik /AXO DRESDEN
Sommerstr. 4
83253 Rimsting, Germany
+4935125089723
www.xhuber.com
markus.kraemer@axo-dresden.de

Incienta Technologie GmbH
Pommernstrasse 22
63110 Rodgau, Germany
+4961066252970
www.incienta.com
vikas@incienta.com

incoatec GmbH
Max-Planck-Str. 2
21502 Geesthacht, Germany
+494152889355
www.incoatec.de
hahn@incoatec.de

iseg Spezialelektronik GmbH
Landstr. 23
01454 Radeberg / OT Rossendorf, Germany
+49351269960
www.iseg-hv.com
sales@iseg-hv.de

Johann Fischer Aschaffenburg Präzisionswerk GmbH & Co. KG
Ruhlandstrasse 72 - 78
63741 Aschaffenburg, Germany
+49602186050
www.jfa.de
hans.fischer@jfa.de

Just Vacuum
Daimlerstr. 17
66849 Landstuhl, Germany
+496371927600
www.justvacuum.com
info@justvacuum.com

Kashiyama Europe GmbH
Leopoldstrasse 244
80807 Munich, Germany
+4989208039455
https://de.kashiyama.com/
keg@kashiyama.com

Leybold GmbH
Bonner Str. 498
50968 Köln, Germany
+4915119772034
www.leybold.com
leander.schulz@leybold.com

LSA GmbH
Äusserer Hofring 11
09429 Wolkenstein, Germany
+4937369172246
https://www.lsa-gmbh.de/
a.strobel@lsa-gmbh.de

MDC Europe
4-7 Carters Lane, Kiln Farm
Milton Keynes, MK11 3ER, United Kingdom
+492305947508
www.mdcvacuum.com
galthoff@mdcvacuum.de

MEWASA AG
Straubstrasse 11A
7323 Vilters-Wangs, Switzerland
+41817204894
www.mewasa.ch
m.gartmann@mewasa.ch

MUEGGE GmbH
Hochstrasse 4-6
64385 Reichelsheim, Germany
+496164930792
www.muegge.de
christian.schloessmann@muegge.de

Nanovak Systeme
Andreas Mattil Talstr.33
67737 Frankelbach, Germany
+4915114304082
www.nanovak-systeme.de
info@nanovak-systeme.de

OmniVac
Hertelsbrunnenring 30
67657 Kaiserslautern, Germany
+496313110740
omnivac@omnivac.de
http://www.omnivac.de
h.ruppender@omnivac.de

Pfeiffer Vacuum GmbH
Berliner Str. 43
35614 Asslar, Germany
+496441023834
www.pfeiffer-vacuum.com
christiane.kempf@pfeiffer-vacuum.de

Physical Electronics GmbH
Salzstrasse 8
85622 Feldkirchen, Germany
+49899627521
www.phi-gmbh.eu
greitenbach@phi-europe.com

Physik Instrumente (PI) GmbH & Co. KG
Auf der Römerstrasse 1
76228 Karlsruhe, Germany
www.physikinstrumente.com
c.schraenkler@pi.de

Phytron GmbH
Industriestasse 12
82194 Gröbenzell, Germany
+498142503168
www.phytron.de
marketing@phytron.de

Picovac
Ziegelhüttenweg 30a
65232 Taunusstein, Germany
+4915731146931
www.picovac.de
Martin.Oertel@picovac.de

Pilz-Optics
Enzianstrasse 29
73485 Unterschneidheim, Germany
+4979668038866
www.pilz-optics.de
Info@pilz-optics.de

PINK GmbH Vakuumtechnik
Gyula-Horn-Str. 20
97877 Wertheim, Germany
+499342872145
www.pink-vak.de
dlang@pink-vak.de

Prevac sp. z o.o.
Raciborska 61 Str
44362 Rogow, Poland
+48602281470
https://www.prevac.eu
a.kuzaj@prevac.eu

ProxiVision GmbH
Stubenwald-Alle 16
64625 Bensheim, Germany
+496251170324
www.proxivision.de
rene.lewinski@proxivision.de

REUTER TECHNOLOGIE GmbH
Röntgenstrasse 1
63755 Alzenau, Germany
+496023504425
www.reuter-technologie.de
contact@reuter-technologie.de

Scienta Omicron GmbH
Limburger Str. 75
65232 Taunusstein, Germany
+491715655817
www.scientaomicron.com
andreas.frank@scientaomicron.com

SmarAct GmbH
Schuette-Lanz-Strasse 9
26135 Oldenburg, Germany
+494418008790
www.smaract.com
schlump@smaract.com

SPECS Nano Oberflaeche Analysis GmbH
Voltastrasse 5
13355 Berlin, Germany
+49304678249340
www.specs-group.com
albana.spirollari@specs.com

Thyracont Vacuum Instruments GmbH
Max-Emanuel-Strasse 10
94036 Passau, Germany
https://thyracont-vacuum.com/
Karin.Schatzberger@thyracont.de

VACGEN Ltd
Unit A, Swallow Business Park, Diamond Drive
Lower Dicker, Hailsham, BN27 4EL, UK
+447826855813
www.vacgen.com
isabelle.moriarty@vacgen.com

VACOM Vakuum Komponenten & Messtechnik GmbH
In den Brückenäckern 3
07751 Grosslöbichau, Germany
+4936418734332
www.vacom.de
linda.schmidt@vacom.de

Vacuum FAB Srl
Via Asilo 74
20010 Cornaredo (MI), Italy
+393487495459
www.vacuumfab.it
guido.giorgi@vacuumfab.it

Vacuum Services Germany
Andreas Mattil Talstr.33
67737 Frankelbach, Germany
+4915114304082
www.vacuumservices-germany.de
info@vacuumservices-germany.de

vakuumfinder.de c/o compoNext GbR
Freiligrathstrasse 35
07743 Jena, Germany
www.vakuumfinder.de
Stine. Heitnann@vakuumfinder.de

Vaqtec Srl
Via Mangiacane 3
12011 Borgo San Dalmazzo (CN), Italy
+393299451836
www.vaqtec.com
r.cometti@vaqtec.com

vaqtec-scientific
Thulestr. 18b
13189 Berlin, Germany
+493078713158
www.vaqtec-scientific.com
melzer@vaqtec-scientific.com

VAT Deutschland GmbH
Zur Wetterwarte 50, Haus 337/G
01109 Dresden, Germany
+4935150193400
http://www.vatvalve.com
shoelzer@vatvalve.com

List of Participants

Ahlberg	Martina	martina.ahlberg@physics.gu.se
Ahsan	Md Sabbir	md.ahsan@helmholtz-berlin.de
Akhmetova	Irina	irina.akhmetova@bam.de
Ali	Hebatallah	hebatallah@fhi-berlin.mpg.de
Allenspach	Stephan	stephan.allenspach@psi.ch
Allibon	John	allibon@ill.fr
Al-Temimy	Ameer	ameer.al-temimy@helmholtz-berlin.de
Amrhein	Tim	tim@adrhinum.de
Andrle	Anna	anna.andrle@ptb.de
Anselmo	Ana	ana.anselmo@helmholtz-berlin.de
Arce	Mauricio D.	mauricio.arce@helmholtz-berlin.de
Arlt	Bastian	bastian.arlt@anton-paar.com
Arlt	Tobias	tobias.arlt@helmholtz-berlin.de
Asyuda	Andika	vv181@uni-heidelberg.de
Avishek	Dey	avishek.dey@open.ac.uk
Bär	Marcus	marcus.baer@helmholtz-berlin.de
Barciszewski	Jakub	agent007@man.poznan.pl
Barthel	Tatjana	tatjana.barthel@helmholtz-berlin.de
Bartkowiak	Maciej	maciej.bartkowiak@helmholtz-berlin.de
Bereswill	Sarah	bereswill@uni-potsdam.de
Beucher	Lucas	lucasbeucher@uni-koblenz.de
Bhattacharya	Biswajit	biswajit.bhattacharya@bam.de
Bienert	Ralf	ralf.bienert@bam.de
Bischof	Daniel	daniel.bischof@physik.uni-marburg.de
Bock-Bierbaum	Tobias	tobias.bock-bierbaum@mdc-berlin.de
Bodenstein-Dresler	Lucas	lucas.bodenstein-dresler@helmholtz-berlin.de
Boin	Mirko	boin@helmholtz-berlin.de
Brandt	Astrid	brandt@helmholtz-berlin.de
Breternitz	Joachim	joachim.breternitz@helmholtz-berlin.de
Britzke	Ralf	ralf.britzke@bam.de
Bronsch	Wibke	wibke.bronsch@fu-berlin.de
Bruno	Giovanni	giovanni.bruno@bam.de
Brzhezinskaya	Maria	maria.brzhezinskaya@helmholtz-berlin.de
Busch	Christian	christian.busch@stud.uni-heidelberg.de
Bzheumikhova	Karina	karina.bzheumikhova@ptb.de
Cabeza Sanchez	Sandra	cabeza@ill.eu
Cappel	Ute	cappel@kth.se
Chen	Dongfeng	dfchenciae@126.com
Chen	Kai	kai.chen@helmholtz-berlin.de
Christian	Gollwitzer	christian.gollwitzer@ptb.de
Cimino	Roberto	roberto.cimino@lnf.infn.iy
Clark	Pip	philippa.clark@helmholtz-berlin.de
Cramm	Stefan	s.cramm@fz-juelich.de
Darowski	Nora	nora.darowski@helmholtz-berlin.de

Dietrich	Paul	paul.dietrich@specs.com
Dong	Kang	kang.dong@helmholtz-berlin.de
Donskyi	Ievgen	idonskyi@gmail.com
Dorn	Alexander E.	andreas.hollmann@helmholtz-berlin.de
Dorn	Katharina	andreas.hollmann@helmholtz-berlin.de
Drescher	Daniela	dreschda@hu-berlin.de
Eckert	Sebastian	eckert@mbi-berlin.de
Esser	Norbert	norbert.esser@isas.de
Falk	Florian	florian.falk@bam.de
Favaro	Marco	marco.favaro@helmholtz-berlin.de
Fedorov	Alexander	a_v_fyodorov_spb@inbox.ru
Feiler	Christian	christian.feiler@helmholtz-berlin.de
Fernández Herrero	Analía	analia.fernandez.herrero@ptb.de
Fijal-Kirejczyk	Izabela	Izabela.Fijal-Kirejczyk@ncbj.gov.pl
Flach	Max	max.flach@helmholtz-berlin.de
Flatken	Marion	marion.flatken@helmholtz-berlin.de
Föhlisch	Alexander	alexander.foehlisch@helmholtz-berlin.de
Fondell	Mattis	mattis.fondell@helmholtz-berlin.de
Förster	Ronald	foerster@helmholtz-berlin.de
Franz	Alexandra	alexandra.franz@helmholtz-berlin.de
Fritsch	Daniel	daniel.fritsch@helmholtz-berlin.de
Fritsch	Katharina	katharina.fritsch@helmholtz-berlin.de
Froideval	Annick	a.froideval@hzdr.de
Frolov	Alexander	alexander_s_frolov@mail.ru
Fürsich	Katrin	k.fuersich@fkf.mpg.de
Gamba	Nadia	gamba.nadia@gmail.com
Garcia Diez	Raul	raul.garcia_diez@helmholtz-berlin.de
Gericke	Eike	eike.gericke@helmholtz-berlin.de
Gerlach	Martin	martin.gerlach@helmholtz-berlin.de
Ghafari	Aliakbar	aa.ghafari@gmail.com
Giangrisostomi	Erika	erika.giangrisostomi@helmholtz-berlin.de
Gless	Christine	christine.gless@helmholtz-berlin.de
Gondek	Lukasz	lgondek@agh.edu.pl
Gorgoi	Mihaela	mihaela.gorgoi@helmholtz-berlin.de
Gottwald	Alexander	alexander.gottwald@ptb.de
Griesche	Axel	axel.griesche@bam.de
Grzimek	Veronika	veronika.grzimek@helmholtz-berlin.de
Guasco	Laura	guasco.laura@gmail.com
Guilherme Buzanich	Ana	ana.buzanich@bam.de
Gurieva	Galina	galina.gurieva@helmholtz-berlin.de
Guttmann	Peter	peter.guttmann@helmholtz-berlin.de
Häbel	Catharina	catharina.haebel@helmholtz.de
Habicht	Klaus	habicht@helmholtz-berlin.de
Hävecker	Michael	mh@fhi-berlin.mpg.de
Hampel	Sven	sven.hampel@tu-clausthal.de
Handick	Evelyn	evelyn.handick@ptb.de
Hanke	Michael	hanke@pdi-berlin.de

Harten	Paul	paul.harten@helmholtz-berlin.de
Hartmann	Claudia	claudia.hartmann@helmholtz-berlin.de
Hauß	Thomas	hauss@helmholtz-berlin.de
Hawly	Tim	tim.hawly@fau.de
He	Huiling	huiling.he@helmholtz-berlin.de
Heilmann	Maria	maria.heilmann@bam.de
Hein	Dennis	dennis.hein@helmholtz-berlin.de
Heinze	Leonie	l.heinze@tu-braunschweig.de
Hellmig	Michael	michael.hellmig@helmholtz-berlin.de
Helms	Ina	ina.helms@helmholtz-berlin.de
Hengge	Michael	michael.hengge@helmholtz-berlin.de
Hennecke	Martin	martin.hennecke@mbi-berlin.de
Hesse	Ronald	rhesse@uni-leipzig.de
Hillier	Heidi T.	heidi.t.hillier@uit.no
Hoehl	Arne	arne.hoehl@ptb.de
Hoell	Armin	hoell@helmholtz-berlin.de
Holfelder	Ina	ina.holfelder@ptb.de
Hollmann	Andreas	andreas.hollmann@helmholtz-berlin.de
Holub-Krappe	Elizabeta	holub-krappe@online.de
Hönicke	Philipp	philipp.hoenicke@ptb.de
Hoser	Andreas	hoser@helmholtz-berlin.de
Hradil	Klaudia	klaudia.hradil@tuwien.ac.at
Jäger	Klaus	klaus.jaeger@helmholtz-berlin.de
Jagodar	Andrea	andrea.jagodar@univ-orleans.fr
Jankowiak	Andreas	andreas.jankowiak@helmholtz-berlin.de
Janowitz	Christoph	christoph.janowitz@b-tu.de
Jauch	Wolfgang	wolfgang.jauch47@t-online.de
Jay	Raphael	raphael.jay@helmholtz-berlin.de
Jianhui	Xu	jianhui.xu@helmholtz-berlin.de
Jimenez	Catalina	catalina.jimenez@helmholtz-berlin.de
Jones	Travis	trjones@fhi-berlin.mpg.de
Juhl	Alice D.	alicedk@bmb.sdu.dk
Jung	Christian	christian.jung@helmholtz-berlin.de
Junghöfer	Tobias	tobias.junghoefer@uni-tuebingen.de
Kachel	Stefan R.	kachels@staff.uni-marburg.de
Kaczerowski	Jürgen	juergen.kaczerowski@zsw-bw.de
Kadletz	Peter M.	peter.kadletz@esss.se
Kafedjiska	Ivona	ivona.kafedjiska@helmholtz-zentrum.de
Karpinsky	Dmitry	dmitry.karpinsky@gmail.com
Karslioglu	Osman	osman.karslioglu@fhi-berlin.mpg.de
Kasatikov	Sergey	sergey.kasatikov@helmholtz-berlin.de
Kaser	Hendrik	hendrik.kaser@ptb.de
Kayser	Yves	yves.kayser@ptb.de
Keiderling	Uwe	keiderling@helmholtz-berlin.de
Keilbach	Andreas	andreas.keilbach@anton-paar.com
Keller	Corina	corina.keller@helmholtz-berlin.de
Kerkhoff	Hans	hans.kerkhoff@ptb.de

Kiefer	Klaus	klaus.kiefer@helmholtz-berlin.de
Kimber	Simon	simon.kimber@u-bourgogne.fr
Kirschner	Hans	hans.kirschner@ptb.de
Kjærvik	Marit	marit.kjaervik@bam.de
Kjellsson	Ludvig	ludvig.kjellsson@physics.uu.se
Klaus	Manuela	klaus@helmholtz-berlin.de
Klein	Roman	roman.klein@ptb.de
Klemke	Bastian	bastian.klemke@helmholtz-berlin.de
Klyushin	Alexander	alexander.klyushin@helmholtz-berlin.de
Kneipp	Janina	janina.kneipp@chemie.hu-berlin.de
Knop-Gericke	Axel	knop@fhi-berlin.mpg.de
Köhler	Ralf	ralf.koehler@lavg.brandenburg.de
Kolbe	Michael	michael.kolbe@ptb.de
Kolenko	Petr	petr.kolenko@fjfi.cvut.cz
Kosinas	Christos	chris.kos.9@gmail.com
Kovacevic	Eva	eva.kovacevic@gmail.com
Krause	Simon	simon.krause@rug.nl
Krähnert	Ralph	ralph.kraehnert@tu-berlin
Krist	Thomas	krist@nanooptics-berlin.com
Kroth	Udo	udo.kroth@ptb.de
Krumrey	Michael	michael.krumrey@ptb.de
Krzyzagorski	Mark	mark.krzyzagorski@helmholtz-berlin.de
Kubin	Markus	markus.kubin@helmholtz-berlin.de
Kuch	Wolfgang	kuch@physik.fu-berlin.de
Kühnholz	Olaf	olaf.kuehnholz@desy.de
Kulow	Anicó	anico.kulow@bam.de
Kumberg	Ivar	ikumberg@zedat.fu-berlin.de
Kumpugdee-Vollrath	Mont	vollrath@beuth-hochschule.de
Kupsch	Andreas	andreas.kupsch@bam.de
Kutukova	Kristina	kristina.kutukova@ikts.fraunhofer.de
Lake	Bella	bella.lake@helmholtz-berlin.de
Lau	Tobias	tobias.lau@helmholtz-berlin.de
Lauermann	Iver	iver.lauermann@helmholtz-berlin.de
Leitner	Torsten	torsten.leitner@helmholtz-berlin.de
Lennartz	Frank	frank.lennartz@helmholtz-berlin.de
Li	Bor	bor.li@helmholtz- berlin.de
Li	Chenghao	chenghao.li@mpikg.mpg.de
Li	Ji	ji.li@helmholtz-berlin.de
Li	Tianfu	litianfu.li@163.com
Linberg	Kevin	kevin.linberg@BAM.de
Lips	Klaus	lips@helmholtz-berlin.de
Litvinenko	Elena	litvin@nf.jinr.ru
Liu	Sunbin	sunbin.liu@fu-berlin.de
Löhmann	Oliver	loehmann@fkp.tu-darmstadt.de
Lounasvuori	Mailis	mailis.lounasvuori@helmholtz-berlin.de
Lüning	Jan	jan.luning@helmholtz-berlin.de
Luo	Chen	chen.luo@tum.de

Lutz	Christian	christian.lutz@tu-clausthal.de
Maaz	Torsten	torsten.maaz@mksinst.com
Magliano	Erica	erica.magliano@helmholtz-berlin.de
Magomedov	Artiom	artiom.magomedov@ktu.lt
Mahmoodinezhad	Ali	ali.mahmoodinezhad@b-tu.de
Mahnke	Heinz-Eberhard	hemahnke@zedat.fu-berlin.de
Mainz	Roland	roland.mainz@helmholtz-berlin.de
Makarova	Anna	anna.makarova@helmholtz-berlin.de
Man	Gabriel	gabriel.man@physics.uu.se
Mani	Deepak	smdeepakmani@gmail.com
Marbina	Stonia	stonia.marbina@helmholtz-berlin.de
Marcano	Lourdes	lourdes.marcano@helmholtz-berlin.de
Marchenko	Dmitry	dmitry.marchenko@helmholtz-berlin.de
Markötter	Henning	henning.markoetter@helmholtz-berlin.de
Martensson	Nils	nils.martensson@physics.uu.se
Martin	Radtke	martin.radtke@bam.de
Martins	Berta	berta.martins@hu-berlin.de
Mascarenhas	Eric Johnn	eric.mascarenhas@helmholtz-berlin.de
Mascotto	Simone	simone.mascotto@chemie.uni-hamburg.de
Mast	Matthias	matthias.mast@helmholtz-berlin.de
Maticiuc	Natalia	natalia.maticiuc@helmholtz-berlin.de
Mayer	Matthew	m.mayer@helmholtz-berlin.de
Menzel	Magnus	magnus.menzel@helmut-fischer.com
Meseck	Atoosa	atoosa.meseck@helmholtz-berlin.de
Michalchuk	Adam	adam.michalchuk@bam.de
Minniberger	Sonja	minniberger@fmp-berlin.de
Moberg	Robert	robert.moberg@romoscientific.se
Mudryk	Karen	karen.mudryk@helmholtz-berlin.de
Mulazzi	Mattia	mattia.mulazzi@helmholtz-berlin.de
Müller	Bernd R.	bernd.mueller@bam.de
Müller	Peter	peter.mueller@ptb.de
Munir	Rahim	rahim.munir@helmholtz-berlin.de
Nandayapa	Edgar	edgar.nandayapa@helmholtz-berlin.de
Nefedov	Alexei	alexei.nefedov@kit.edu
Neppl	Stefan	stefan.neppl@helmholtz-berlin.de
Neuber	Sven	sven.neuber@uni-greifswald.de
Nie	Kaiqi	kaiqi.nie@helmholtz-berlin.de
Niederhausen	Jens	jens.niederhausen@helmholtz-berlin.de
Novakovic	Nina	nina.novakovic@helmholtz-berlin.de
Ogor	Oskar	oskar.ogor@ptb.de
Osenberg	Markus	markus.osenberg@helmholtz-berlin.de
Osmic	Emir	e_osmic@hotmail.com
Oßwald	Oliver	oliver.osswald@phys.chemie.uni-giessen.de
Ovsyannikov	Ruslan	ovsyannikov@helmholtz-berlin.de
Paulin	Mariano A.	mariano.paulin@helmholtz-berlin.de
Paustian	Wolfgang	wolfgang.paustian@ptb.de
Pechimuthu	Dinesh	dineshpechimuthu1408@gmail.com

Peinl	Florian	florian.peinl@ptb.de
Petit	Tristan	tristan.petit@helmholtz-berlin.de
Pfaff	Torben	torben.pfaff@phys.Chemie.uni-giessen.de
Pflüger	Mika	mika.pflueger@ptb.de
Poerschke	Rainer	rainer.poerschke@freenet.de
Prashanthan	Karunanantharajah	k.prashanthan@helmholtz-berlin.de
Pratsch	Christoph	cpratsch@fhi-berlin.mpg.de
Prieto	Mauricio J.	prieto@fhi-berlin.mpg.de
Prokes	Karel	prokes@helmholtz-berlin.de
Prokhnenko	Oleksandr	prokhnenko@helmholtz-berlin.de
Rabchinskii	Maksim	rabchinskii@mail.ioffe.ru
Radnik	Jörg	joerg.radnik@bam.de
Radu	Florin	florin.radu@helmholtz-berlin.de
Radu	Ilie	radu@mbi-berlin.de
Raoux	Simone	simone.raoux@helmholtz-berlin.de
Reehuis	Manfred	reehuis@helmholtz-berlin.de
Reinholz	Uwe	uwe.reinholz@bam.de
Richter	Tobias	tobias.richter@esss.se
Ripepi	Davide	d.ripepi@tudelft.nl
Risch	Marcel	marcel.risch@helmholtz-berlin.de
Ritter	Eglof	eglof.ritter@hu-berlin.de
Rolf	Fliegauf	rolf.fliegauf@ptb.de
Roske	Johann J.	jonasroske@zedat.fu-berlin.de
Rötger	Antonia	antonia.roetger@helmholtz-berlin.de
Rulev	Alexey	a.rulev@fmlab.ru
Rupp	Axel	rupp-a@helmholtz-berlin.de
Ruppenthal	Lukas	lukas.ruppenthal@chemie.uni-marburg.de
Saadeh	Qais	qais.saadeh@ptb.de
Sajedi	Maryam	maryam.sajedi@helmholtz-berlin.de
Salami	Zanyar	zanyar.salami@helmholtz-berlin.de
Samartzis	Alexandros	alexandros.samartzis@helmholtz-berlin.de
Sauer	Olaf-Peter	sauer@helmholtz-berlin.de
Schedel	Thomas	schedel-niedrig@helmholtz-berlin.de
Schellenberger	Martin	martin.schellenberger@helmholtz-berlin.de
Schiwietz	Gregor	schiwietz@ helmholtz-berlin.de
Schlebrowski	Torben	schlebrowski@uni-koblenz.de
Schlegel	Moritz-Caspar	moritz-caspar.schlegel@bam.de
Schmidt	Jan-Simon	jan-simon.schmidt@helmholtz-berlin.de
Schmidt	Thomas	schmidtt@fhi-berlin.mpg.de
Schmitz	Detlef	schmitz@helmholtz-berlin.de
Schmitz-Antoniak	Carolin	c.schmitz-antoniak@fz-juelich.de
Schneidewind	Astrid	astrid.schneidewind@frm2.tum.de
Scholz	Frank	frank.scholz@desy.de
Scholze	Frank	frank.scholze@ptb.de
Schröder	Vincent	schroedv@hu-berlin.de
Schröder-Smeibidl	Birgit	admin.vorstand@dife.de
Schulz	Christian	schulz-c@helmholtz-berlin.de

Schumann	Frank Oliver	schumann@mpi-halle.de
Schwarz	Lisa	lisa.schwarz@helmholtz-berlin.de
Schwarzkopf	Olaf	olaf.schwarzkopf@helmholtz-berlin.de
Sear	Michael	michael.sear@helmholtz-berlin.de
Seidel	Robert	robert.seidel@helmholtz-berlin.de
Seidlhofer	Beatrix	beatrix-kamelia.seidlhofer@helmholtz-berlin.de
Sepulveda	Anderson	anderson.sepulveda@ufabc.edu.br
Serrano Munoz	Itziar	itziar.serrano-munoz@bam.de
Shams	S. Fatemeh	f.shams@fz-juelich.de
Siewert	Frank	frank.siewert@helmholtz-berlin.de
Sikolenko	Vadim	vadim.sikolenko@jinr.ru
Sill	Annekatrin	annekatrin.sill@uni-greifswald.de
Siouris	Ioannis	jsiou@pme.duth.gr
Sivkov	Viktor	sivkovvn@mail.ru
Skroblin	Dieter	dieter.skroblin@ptb.de
Smarsly	Bernd	smarsly@uni-giessen.de
Smekhova	Alevtina	alevtina.smekhova@helmholtz-berlin.de
Smirnov	Dmitry	dmitry.smirnov@helmholtz-berlin.de
Smith	Joel	jasmith3@sheffield.ac.uk
Sokolov	Andrey	andrey.sokolov@helmholtz-berlin.de
Soltwisch	Victor	victor.soltwisch@ptb.de
Sprengel	Maximilian	maximilian.sprengel@bam.de
Staier	Florian	florian.staier@helmholtz-berlin.de
Starr	David	david.starr@helmholtz-berlin.de
Steffien	Michael	michael.steffien@helmholtz-berlin.de
Steigert	Alexander	alexander.steigert@helmholtz-berlin.de
Streeck	Cornelia	cornelia.streeck@ptb.de
Strunskus	Thomas	ts@tf.uni-kiel.de
Süllow	Stefan	s.suellow@tu-bs.de
Sun	Kai	ksun@sina.com
Svensson	Svante	svante.svensson@physics.uu.se
Szczerba	Daniel	daniel_szczerba@etu.u-bourgogne.fr
Taberman	Helena	helenataberman@helmholtz-berlin.de
Tanase	Liviu C.	tanase@fhi-berlin.mpg.de
Tegeler	Erich	erich.tegeler@gmx.net
Temst	Kristiaan	kristiaan.temst@kuleuven.be
Terborg	Ralf	ralf.terborg@bruker.com
Thornagel	Reiner	reiner.thornagel@ptb.de
Timm	Martin	martin.timm@helmholtz-berlin.de
Többens	Daniel	daniel.toebbens@helmholtz-berlin.de
Torres	Jorge	jorge.torres@fu-berlin.de
Tötzke	Christian	christian.toetzke@uni-potsdam.de
Tovar	Michael	tovar@helmholtz-berlin.de
Tran	Van K.	tran.khanh@helmholtz-berlin.de
Trapp	Marcus	marcus.trapp@grs.de
Treimer	Wolfgang	treimer@beuth-hochschule.de
Trepka	Heiko	h.trepka@fkf.mpg.de

Unger	Wolfgang	wolfgang.unger@bam.de
Unterumsberger	Rainer	rainer.unterumsberger@ptb.de
Valenta	Donald	donald.valenta@helmholtz-berlin.de
van der Merwe	Marianne	marianne.vdm@helmholtz-berlin.de
Viefhaus	Jens	jens.viefhaus@helmholtz-berlin.de
Visser	Dirk	d.visser@lboro.ac.uk
Vollmer	Antje	antje.vollmer@helmholtz-berlin.de
Wagner	Andreas	andreas.wagner@bam.de
Wählisch	André	andre.waehlisch@ptb.de
Wallacher	Dirk	dirk.wallacher@helmholtz-berlin.de
Wang	Zhenyu	zhenyu.wang@helmholtz-berlin.de
Wartner	Garlef	garlef.wartner@helmholtz-berlin.de
Weber	Gert	gert.weber@helmholtz-berlin.de
Weiss	Manfred	msweiss@helmholtz-berlin.de
Wellert	Stefan	s.wellert@tu-berlin.de
Wendt	Robert	robert.wendt@helmholtz-berlin.de
Wenisch	Robert	robert.wenisch@helmholtz-nerlin.de
Wernet	Philippe	philippe.wernet@physics.uu.se
Wibowo	Enggar P.	enggar.wibowo@helmholtz-berlin.de
Wiedemann	Dennis	dennis.wiedemann@chem.tu-berlin.de
Wiedenmann	Albrecht	alwiedenmann@gmx.de
Williams	Alan	alan.williams@wallacecollection.org
Wilpert	Thomas	wilpert@helmholtz-berlin.de
Wintz	Sebastian	wintz@is.mpg.de
Witte	Ulrike	witte@helmholtz-berlin.de
Wollenhaupt	Jan	jan.wollenhaupt@helmholtz-berlin.de
Wolter	Bettina	bettina.wolter@helmholtz-berlin.de
Wong	Deniz	deniz.wong@helmholtz-berlin.de
Würges	Jochen	jochen.wuerges@desy.de
Wüstner	Daniel	wuestner@bmb.sdu.dk
Xiao	Jie	jie.xiao@helmholtz-berlin.de
Yivlialin	Rossella	rossella.yivlialin@helmholtz-berlin.de
Yogi	Arvind K.	yogi.arvind2003@gmail.com
Yusenko	Kirill	kirill.yusenko@bam.de
Zabel	Hartmut	hartmut.zabel@rub.de
Zerbe	Silvia	silvia.zerbe@helmholtz-berlin.de

Procedures 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 User Committee 2020 is
23. November 2019 [00:01] – **06. December 2019** [23:59]

Eligible users are defined as users of HZB's large-scale facilities, BER II and BESSY II, who have been actively registered on 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 by email by the User Committee election Committee. In order to be able to vote, the users must be registered in GATE.

List of candidates

Eva Kovacevic	GREMI - Université d'Orléans, France	Physicist Methods: NEXAFS, XPS, FTIR Areas of interest: Plasma, thin films, nano structures, Carbon, polymers

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:

Harald Schmidt	Technische Universität Clausthal	Member of the User Commitee
Olaf Schwarzkopf	HZB	Representative of the Scientific Director's Office
Beatrix-Kamelia Seidlhofer	HZB	Representative of the HZB User Coordination

Friends of Helmholtz-Zentrum Berlin e.V.

The purpose of the Association of Friends of Helmholtz-Zentrum Berlin 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

An den Vorstand
Freundeskreis Helmholtz-Zentrum Berlin e.V.
Albert-Einstein Straße 15
12489 Berlin
Germany

Tel.: +49-30-8062 - 12901
Fax.: +49-30-8062 - 12920
e-mail: freundeskreis(at)helmholtz-berlin.de
Internet: http://www.helmholtz-berlin.de/freundeskreis

Mitgliedschaft

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

Membership

Herewith I apply for admission to the Association Friends of Helmholtz-Centre Berlin

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

Die jährlichen Mitgliedsbeiträge betragen zur Zeit für natürliche Personen EUR 40,-, für juristische Personen EUR 150,-, EUR 100,- oder EUR 50,-, für Studenten EUR 10,-. / The regular annual membership fees amount to EUR 40,- for natural persons, EUR 150,–/100,-/50,- for legal entities, EUR 10,- for students.

Art der Person: / Character of person: natural person _____ legal entity _____
Mitgliedsbeitrag : / Membership fees: Euro _____

Im Rahmen freiwilliger Höherstufung/ voluntary upgrading: Euro _____

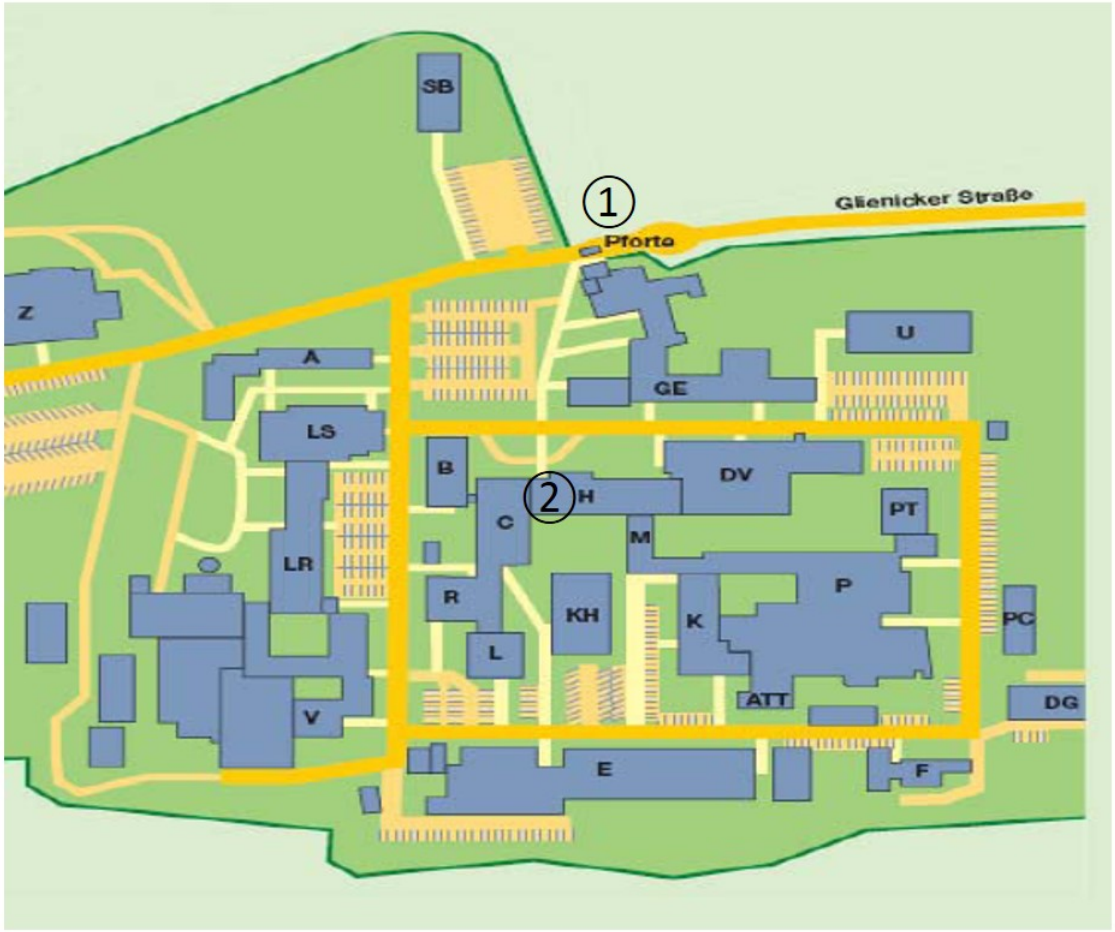
Datum: / date: Unterschrift: / signature:

This page is intentionally left blank for your notes.

This page is intentionally left blank for your notes.

This page is intentionally left blank for your notes.

Helmholtz-Zentrum Berlin
Lise-Meitner Campus
Wannsee

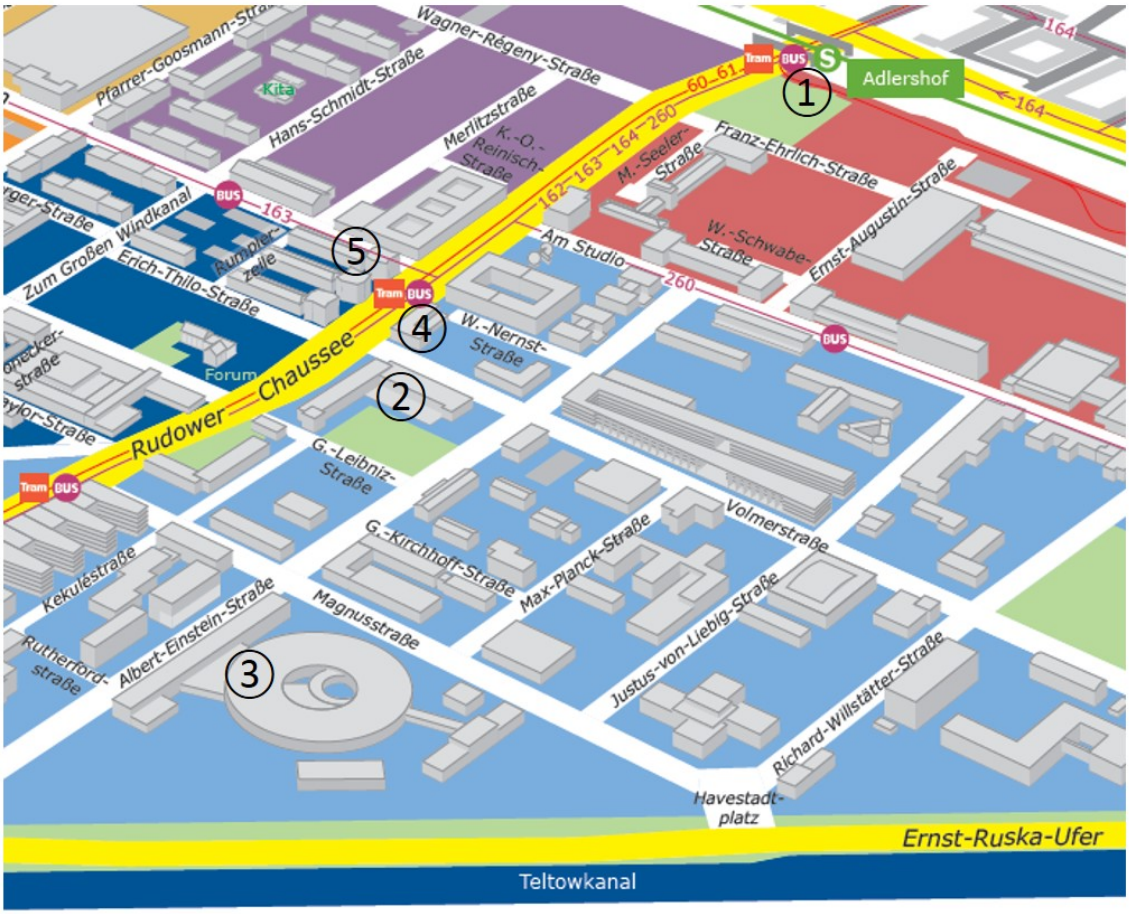


1 Main entrance
2 Lecture building (H): LMC-Foyer
Cafe Jahn
Lecture Hall

BER II
Hahn-Meitner-Platz 1
14109 Berlin

tel +49 (0)30 8062-42304
neutrons@helmholtz-berlin.de

Helmholtz-Zentrum Berlin
Wilhelm-Conrad-Röntgen Campus
Adlershof



① Train Station Adlershof
② Wista centre: Registration
Bunsen Auditory
Vendor Exhibition
③ BESSY II Storage Ring Hall: Poster Session

Hotels:
④ Dorint
⑤ Airporthotel

BESSY II
Albert-Einstein-Str. 15
12489 Berlin
tel +49 (0)30 8062-12931
photons@helmholtz-berlin.de

ONE VOICE FOR THE BRIGHTEST SCIENCE

lightsources.org is the result of a collaboration between communicators from light source facilities around the world.

24 organisations

Representing 29 facilities worldwide, 22 synchrotrons and 7 FELs

40,000 articles

Published by our user community between 2013 and 2017

6,300 protein structures

Deposited by our user community into the worldwide Protein Data Bank in 2018

WWW.LIGHTSOURCES.ORG

A single platform for:

- **News and science highlights**
- **Proposal deadlines**
- **Career opportunities, PhD and postdoc positions**
- **Workshop and conference calendars**
- **Profile page for each facility**

SIGN UP TO OUR WEEKLY NEWSLETTER!

www.lightsources.org
@lightsources
lightsources.org
lightsources_org

A worldwide voice for the light source user community

KEEP UP TO DATE WITH OUR MONTHLY NEWSLETTER

- news for users
- jobs
- events & workshops
- science highlights

Subscribe here:

www.hz-b.de/newsletter-en

HZB Helmholtz Zentrum Berlin

Next deadline for submission:

1st March 2020

Call for Proposals 2020/II

HZB kindly invites you to submit proposals for the next allocation period from August 2020 to February 2021 for BESSY II.

Beamtime applications may only be submitted via the General Access Tool GATE:

http://hz-b.de/gate

For guidance in writing a proposal, please refer to the online guide for beamtime application:

http://hz-b.de/beamguide

http://hz-b.de/proposals