

FOCUSSING ENERGY REALIZING VISIONS



THz TO SOFT X-RAY WORKSHOP

BESSY II

December 7 - 8, 2015
Berlin-Adlershof

Dear participant,

HZB kindly welcomes you to our foresight workshop “THz-to-Soft X-Rays”.

Covering resonance energies of oxygen, nitrogen, carbon, or 3d transition metals, soft x-ray photons provide element specificity and unravel the local electronic structure of materials in energy materials research, magnetism, spintronics, electron correlations, (surface) chemistry and catalysis. VUV photoelectron spectroscopy is at the heart of connecting electronic band structure with macroscopic properties. Infrared light is especially helpful to investigate biological systems as well as vibrational, structural and electronic properties of liquids, solids, surfaces and thin layers while coherent THz radiation is unique for magnetic resonance spectroscopy.

BESSY II offers a broad range of photon energies to study materials relevant to the big societal challenges related to energy conversion and storage, energy-efficient information technology, as well as catalysis and life sciences.

The scope of this workshop is to present achievements and perspectives of these various fields, and to foster discussion about future requirements on the source and instrumentation to exploit at best synchrotron radiation over the whole range from THz to soft x-rays.

We invite you to discuss these opportunities with us at the workshop.

The Workshop “THz-to-Soft X-Rays II” is the fourth in a series of foresight workshops at BESSY II which are designed to establish a continuous discussion platform for future projects and research activities in concert with current and future users from universities, research institutes, and industry. The aim of the dialogue is to identify future scientific fields as well as expectations, needs, and requirements for cutting edge science with synchrotron radiation.

We hope that this workshop will stimulate your interest in future developments at BESSY II and initiate fruitful discussions and new experiments and collaborations. Thank you all for joining us and enjoy the meeting.

Sincerely,

A handwritten signature in black ink, appearing to read 'A. Pyzalla', written in a cursive style.

Prof. Dr.-Ing. Anke Kaysser-Pyzalla
Scientific Director and Chief Executive

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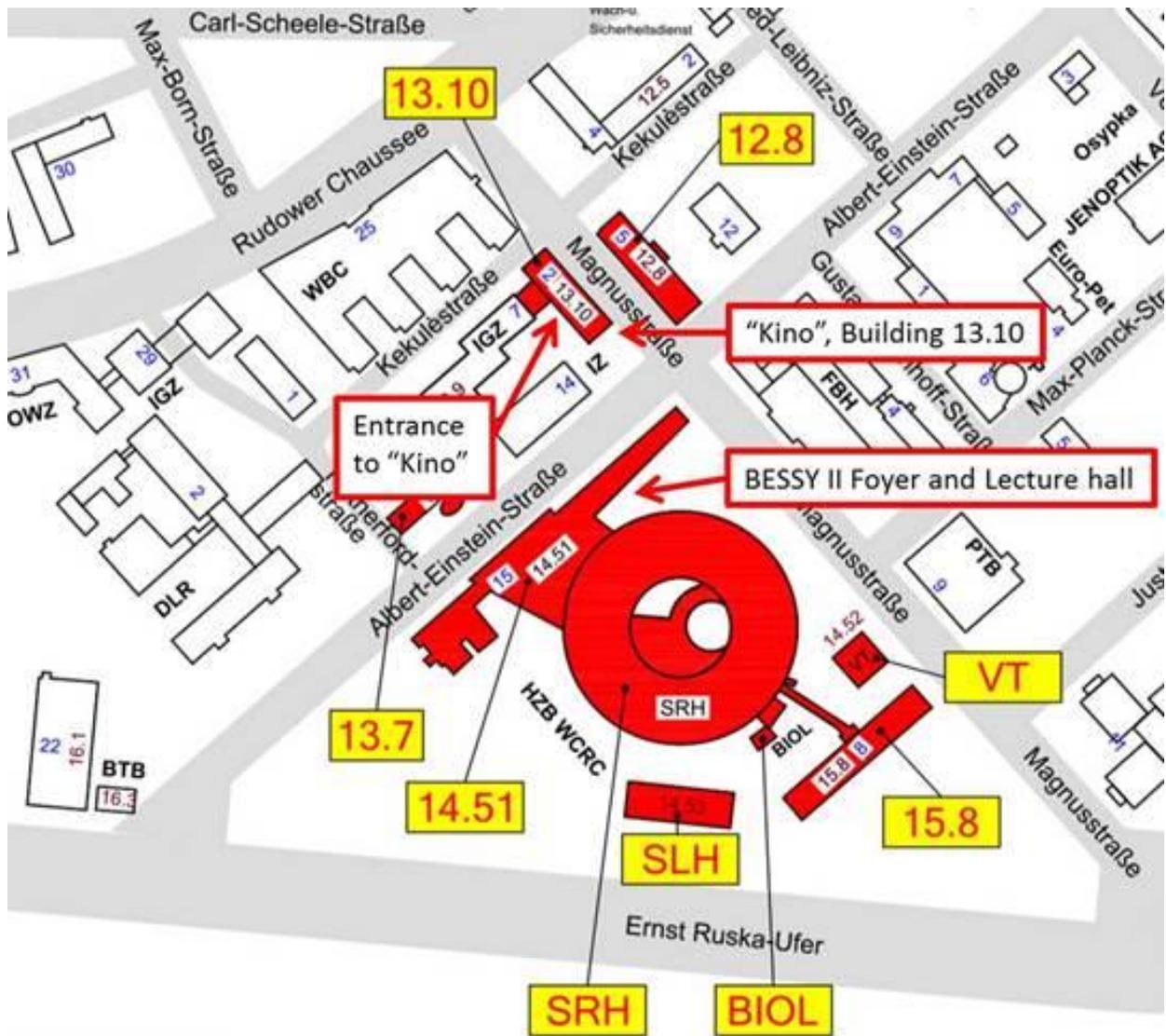
THz to Soft X-ray Workshop

(7/8. Dec. 2015)

First Day, Monday 7 th of December		
Registration (BESSY II Foyer)		8:45
Welcome	Andreas Jankowiak, <i>HZB</i>	9:15 – 9:30
Overview Talks (BESSY II Lecture Hall)		9:30 – 13:00
Energy Research	Maya Kiskinova, <i>Elettra-Sincrotrone Trieste</i>	9:30 – 10:00
Solution Chemistry	Steven Bradforth, <i>University of Southern California</i>	10:00 – 10:30
Magnetism	Gerrit van der Laan, <i>Diamond Light Source</i>	10:30 – 11:00
Coffee Break		11:00 – 11:30
Correlated Materials	Bernd Büchner, <i>IFW Dresden</i>	11:30 – 12:00
Life Science	Peter Hegemann, <i>HU Berlin</i>	12:00 – 12:30
Spintronics	Jean-Marc Triscone, <i>University of Geneva</i>	12:30 – 13:00
Lunch Break (BESSY II Foyer)		13:00 – 14:00
Topical Sessions		14:00 – 18:00
Energy Research BESSY II Lecture Hall	Magnetism "Kino" Building 13.10	
Håkan Rensmo, <i>Uppsala Universitet</i>	Stephen Hill, <i>Florida State University</i>	14:00 – 14:30
Lada Yashina, <i>Moscow State University</i>	Wolfgang Kuch, <i>FU Berlin</i>	14:30 – 15:00
Antoine Kahn, <i>Princeton University</i>	Martin Aeschlimann, <i>TU Kaiserslautern</i>	15:00 – 15:30
Coffee Break		15:30 – 16:00
Arno Smets, <i>TU Delft</i>	Julie Karel, <i>MPI for Chemical Physics of Solids</i>	16:00 – 16:30
Artur Braun, <i>EMPA</i>	Mathias Kläui, <i>JGU Mainz</i>	16:30 – 17:00
Georg Held, <i>Diamond Light Source</i>	Christian Tusche, <i>Forschungszentrum Jülich</i>	17:00 – 17:30
Ideas, Suggestions and Requirements concerning Beam, Instrumentation and Sample Environment		17:30 – 18:00
Poster Session - Snacks (BESSY II Foyer)		18:00

Second Day, Tuesday 8th of December		
Topical Sessions		9:00 – 11:45
Spintronics BESSY II Lecture Hall	Solution Chemistry "Kino" Building 13.10	
Gerd Schönhense, <i>JGU Mainz</i>	Richard Buchner, <i>Universität Regensburg</i>	9:00 – 9:30
Kai Rosnagel, <i>CAU Kiel</i>	Matthew Brown, <i>ETH Zürich</i>	9:30 – 10:00
Coffee Break		10:00 – 10:20
Eli Rotenberg, <i>Lawrence Berkeley National Laboratory</i>	Yoshihisa Harada, <i>University of Tokyo</i>	10:20 – 10:50
Vladimir Strocov, <i>Paul Scherrer Institute</i>	Olle Björneholm, <i>Uppsala Universitet</i>	10:50 – 11:20
Ideas, Suggestions and Requirements concerning Beam, Instrumentation and Sample Environment		11:20 - 11:45
Topical Sessions		11:45 – 12:45
Correlated Materials BESSY II Lecture Hall	Life Science "Kino" Building 13.10	
Ralph Ernstorfer, <i>Fritz-Haber-Institut</i>	Serena de Beer, <i>MPI für Chemische Energiekonversion</i>	11:45 – 12:15
Michael Först, <i>MPI for the Structure and Dynamics of Matter</i>	Mark Sherwin, <i>University of California</i>	12:15 – 12:45
Lunch Break (BESSY II Foyer)		12:45 – 13:45
Sergey Borisenko, <i>IFW Dresden</i>	Jan Kern, <i>Lawrence Berkeley National Laboratory</i>	13:45 – 14:15
Hao Tjeng, <i>MPI for Chemical Physics of Solids</i>	Andrea Lübcke, <i>Max-Born-Institut</i>	14:15 – 14:45
Ideas, Suggestions and Requirements concerning Beam, Instrumentation and Sample Environment		14:45 – 15:05
Coffee Break (BESSY II Foyer)		15:05 – 15:30
Into the Future (BESSY II Lecture Hall)		
BESSY II Accelerator Instrumentation	Andreas Jankowiak, <i>HZB</i>	15:30 – 16:00
BESSY II Photon Science Instrumentation	Alexander Föhlisch, <i>HZB</i>	16:00 – 16:30
General Discussion and Summary		16:30 – 17:00
End of the Workshop		17:00
Visit of BESSY II		

Site plan



Lecture hall:

Overview talks, Sessions Energy Research, Spintronics, Correlated Materials and Into the Future

Kino:

Sessions Magnetism, Solution Chemistry and Life Science

BESSY II Foyer:

Poster Session, Lunch, Snacks

Abstracts of the Overview Talks

Monday, 7th of December

Location: BESSY II Lecture hall

Microscopic Insights on the Morpho-chemical Evolution of Functional Components in Electrochemical Devices

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Notwithstanding the environmental appeal of electrochemical devices, their widespread applications are still hindered by ‘material’ problems, chiefly related to the durability of crucial functional components. Important missing chains are in the molecular level understanding of some key factors determining morpho-chemical coupling during electrochemical processes, which has pushed the development of appropriate methods for characterization of material evolution at functionally relevant length and time scales. In this respect the complementary capabilities of synchrotron-based soft X-ray scanning microscopes, in terms of imaging, spectroscopy, spatial and time resolution and variable probing depths, combined with the development of simplified versions of cells and devices, have opened unique opportunities to characterize these complex systems *in-situ* with sub-micrometer lateral resolution ^[1]. The achievements in this respect will be illustrated by selected studies exploring the variations in morphology and chemical state of key functional constituents as a function of growth ^[2] or operating conditions ^[3]. Ongoing efforts for pushing the lateral resolution by implementing ptychography and working under realistic ambient conditions will be outlined and briefly discussed.

References:

[1] B. Bozzini et al, Chemistry A European Journal 18, 10196 (2012).

[2] P. Bocchetta et al, ACS Appl. Mater. Interfaces 6, 19621–19629 (2014).

[3] B. Bozzini et al, Scientific Reports, DOI: 10.1038/srep02848 (2013).

Photoelectron Spectroscopy to Probe Bulk and Interface Chemistry in Aqueous Solution

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Understanding how the electronic structure of a water molecule, or a solute dissolved in water, is intricately bound up with the arrangement of the liquid water network provides insight into how chemical reactions are influenced by the environment in which they take place. Techniques that can resolve the nanoscale structure around a solute ion in bulk solution or at an aqueous interface can provide new insights into chemical mechanisms at play in catalysis and biochemistry and hold promise for probing chemistry of solutes to varying depths below the water/gas interface, of significance for atmospheric processes.

In this overview talk, I will provide illustrations of these interconnections including those from our own work using photoelectron spectroscopy to uncover how electronic structure changes during bond breaking, proton transfer and redox reactions.^[1,2]

Acknowledgments: This work is made possible by financial support from the US National Science Foundation under CHE-1301465 as well as beam time granted by HZB Berlin. R. Seidel was supported with a DFG Postdoctoral Fellowship.

References:

[1] Pluhařová, E.; Schroeder, C.; Seidel, R.; Bradforth, S. E.; Winter, B.; Faubel, M.; Slavíček, P.; Jungwirth, P. *J. Phys. Chem. Lett.* 2013, *4*, 3766–3769.

[2] Schroeder, C. A. et al., *J. Am. Chem. Soc.* 2015, *137*, 201–209.

Opportunities of x-ray magnetic spectroscopy

Gerrit van der Laan

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This talk will discuss what kind of information one can obtain using polarized x-ray absorption and related spectroscopies on magnetic materials.

Previously, information processing technology purely relied on charge-based devices, ranging from the old vacuum tube to today's microchips. However the quantum properties of the electron known as spin can be used as a tag for the electron path and is the cornerstone of magnetism. Microelectronic devices that operate by using the spin are a nascent multibillion dollar industry and may lead in the near future to quantum computing. Novel magnetic materials can be tailored thanks to the application of polarized synchrotron radiation. Core level spectroscopy offers unique element-specific information, not obtainable by other techniques such as neutron scattering. Examples from research where polarized synchrotron radiation has provided further understanding include x-ray magnetic circular and linear dichroism, dichroic photoemission, resonant magnetic x-ray scattering, and photoelectron emission microscopy, x-ray holography on magnetic materials such as ferromagnetic semiconductors, giant magnetoresistance materials, magnetic tunnel junctions, half metallic systems, spin valves, exchange bias springs, frustrated magnets, multiferroics, topological insulators, skyrmions, biomagnets, magnetic nanostructures, and self-assembled domain structures. Third generation facilities have made it possible to use the phase coherence and time structure of the x-rays, giving access to the local magnetic order and to the spin dynamics. The novel synchrotron-radiation-based technique of x-ray detected ferromagnetic resonance (XFMR) allows us to measure FMR in a time-resolved and element-specific way and to obtain the phase of the magnetic precession.

Correlated Metals: Electronic Order, Orbitals and Hund's Coupling

Bernd Büchner

Institut für Festkörperforschung, IFW Dresden
Institut für Festkörperphysik, TU Dresden

In recent years it became apparent that orbital degrees of freedom are not only important for the physics of magnetic insulators but also for that of many itinerant electron systems. In my talk I will flash some recent examples and then discuss in more detail the physics of Fe based superconductors and related compounds. In these systems orbitals are crucial for density wave instabilities and so-called nematic order. Moreover, the strength and relevance of electronic correlations in these multi-orbital systems are controlled by Hund's rule coupling. Based on ARPES measurements I will argue that the class of transition metal pnictides may serve as model systems to control and understand correlation effects in metals with intermediate strength of electronic correlations.

Spectroscopy of light triggered sensory proteins

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Sensory photoreceptors, for example the light-triggered ion channel Channelrhodopsin or light-activated enzymes as Phototropin, are widely distributed in green algae and other microorganism^[1]. In these proteins light absorption causes stepwise structural alterations at timescales from nanoseconds to milliseconds that convert these proteins from an inactive into an active state^[2]. Owing to these properties they are frequently used as optogenetic tools in neurophysiology and biomedicine^[3]. The photocycle of these proteins can be studied by UV/Vis and infrared spectroscopy *in situ*. Especially the mid-infrared spectral region is widely used to obtain such structural information. When dynamic systems are to be investigated, the commonly applied time-resolved IR-spectroscopy utilizing the fourier-transform infrared (FTIR) method allows time-resolutions down to nanoseconds but an essential prerequisite is that the experiment can be repeated in exactly the same way thousands of time, connoting that the systems under investigation are cyclic within milliseconds. This is not the case for many sensory photoreceptors and energy storing photosystems. We report about a novel approach that allows for analyzing non-reversible photoreactions in single shot experiments. Highly brilliant synchrotron infrared radiation, a dispersive Féry-spectrograph and a modern focal-plane array detector are utilized for single-shot measurements in the microsecond time-regime^[4,5]. First commissioning results of this spectrometer will be presented which will find wide applications in life sciences as well as in other fields like energy science.

References:

- [1] Nagel, G., Ollig, D., Fuhrmann, M., Kateriya, S., Musti, A. M., Bamberg, E., and Hegemann, P. (2002) *Science*. 296
 - [2] Schneider, F., Grimm, C., and Hegemann, P. (2015) *Annu. Rev. Biophys.* 44
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 - [5] Ritter, E., Puskar, L., Bartl, F. J., Aziz, E. F., Hegemann, P., and Schade, U. (2015) *Front. Mol. Biosci.* 2
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Magnetic coupling through lanthanum nickelate in non-metallic (111) LaMnO₃/LaNiO₃ superlattices

M. Gibert¹, M. Viret^{1,2}, S. Catalano¹, J. Fowlie¹, P. Zubko³, N. Jaouen⁴, J.-M. Tonnerre⁵, and J.-M. Triscone¹

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Perovskite nickelates (RNiO₃, RE = Rare Earth) are fascinating materials, well known for their metal to insulator transition (MIT) and unique antiferromagnetic (AFM) ground state ^[1]. In this presentation, I will first discuss how one can control the MIT and the magnetic properties of high quality epitaxial nickelate films through a variety of techniques ^[2-6]. I will then describe our work on heterostructures containing LaNiO₃ – the only member of the family that is metallic and paramagnetic in the bulk down to low temperature – and ferromagnetic LaMnO₃. In this system we observed an unusual exchange bias in [111] oriented (LaNiO₃)/(LaMnO₃) superlattices ^[7] and an antiferromagnetic interlayer exchange coupling above the blocking temperature of the exchange biased state specifically in 7 unit cells / 7 unit cells superlattices. The antiferromagnetic coupling is attributed to the presence of a (1/4, 1/4, 1/4) wavelength AFM structure in LaNiO₃. The complex exchange bias observed in this (LaNiO₃)/(LaMnO₃) system is explained in this context also considering the presence of two types of interfaces ^[8].

References:

- [1] ML. Medarde, *Journal of Physics: Condensed Matter*, **9**, 1679 (1997).
- [2] R. Scherwitzl *et al.*, *Advanced Materials* **22**, 5517 (2010).
- [3] S. Catalano *et al.*, *Appl. Phys. Lett. Mat.* **2**, 116110 (2014).
- [4] S. Catalano *et al.*, *Appl. Phys. Lett. Mat.* **3**, 062506 (2015).
- [5] A. Caviglia *et al.*, *Phys. Rev. Lett.* **108**, 136801 (2012).
- [6] M. Först *et al.*, *Nat. Mat.* **14**, 883 (2015).
- [7] M. Gibert *et al.*, *Nat. Mat.* **11**, 195 (2012).
- [8] M. Gibert *et al.*, *Nanoletters* in press (2015).

Abstracts of the Energy Research Session

Monday, 7th of December

Location: BESSY II Lecture hall

Understanding Solar Cell Interfaces Using Electron Spectroscopy

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New materials and material combinations for the use in mesoscopic solar cells and Li-ion batteries has been subject of substantial academic and commercial research over the last decades. The efficiency of the conversion process in these systems is largely dependent on the properties of the interfacial region including material organisation as well as on energy matching between the different condensed phases including inorganic materials, molecular materials and electrolytes. Insight into the material organisation and electronic structure is therefore crucial in order to understand and optimize the function. X-ray based techniques such as photoelectron spectroscopy (PES) are powerful for obtaining such information at an atomic level due to the possibility for element specificity. This contribution reviews some of our PES results and developments for understanding energy related materials specifically including mesoscopic solar cells. Specifically it will be shown how combinations of soft and hard X-ray photoelectron spectroscopy can be used to experimentally understand the electronic structure at interfaces. The talk contains examples targeting energy matching in perovskite solar cells ^[1-3].

References:

- [1] Johansson, E. Lindblad, R., Siegbahn H., Hagfeldt, A., Rensmo, H., Interface Atomic and Electronic Structure in Dye-Sensitized Nanostructured Solar Cells, *ChemPhysChem*, 15, 2014, 1006
 - [2] Lindbad, R., Bi, D., Park, B.-w., Oscarsson, J., Gorgoi, M., Siegbahn, H., Odelius, M., Johansson, E.M.J., and Rensmo, H., Electronic Structure of TiO₂/CH₃NH₃PbI₃ Perovskite Solar Cell Interfaces. *Journal of Physical Chemistry Letters*, 5, 2014, 648
 - [3] Lindblad R; Jena NK; Philippe B; Oscarsson J; Bi D; Lindblad A; Mandal S; Pal B; Sarma DD; Karis O; Siegbahn H; Johansson EMJ; Odelius M; Rensmo H. Electronic Structure of CH₃NH₃PbX₃ Perovskites: Dependence on the Halide Moiety. *Journal of Physical Chemistry C*. 2015;119(4):1818-25
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Probing operating electrochemical interfaces by soft X-rays

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The operation of all electrochemical energy-related systems, such as supercapacitors, batteries, fuel cells, etc. depends largely on the processes occurring at electrochemical interfaces at which charge separation and chemical reactions occur. Evolution of structure and composition at the interface between electrodes and electrolytes affects all the device's functional parameters including power and long-term performance stability. The analytical techniques capable of exploring the interfaces are still very limited, and more often only *ex situ* studies are performed. This sometimes leads to a loss of important pieces of the puzzle, hindering the development of novel technologies, as in many cases intermediates and electrochemical reaction products cannot be “quenched” for post-process analyses. Moreover, real electrochemical interfaces are buried, so that they are inaccessible directly to the common surface science tools. At the same time the bulk sensitive techniques suffer from a minor contribution of the interface to the signal. There are following approaches, which potentially address the problem:

1. Attempts to implement traditional surface-sensitive tools like photoemission with increased probing depth and/or minimized electrode or electrolyte layer thickness.
2. Application of techniques with intrinsic interface sensitivity (surface X-ray scattering, vibrational sum frequency generation spectroscopy, surface-enhanced Raman spectroscopy).
3. Efforts to enhance the surface sensitivity of traditionally “bulk-sensitive” techniques such as X-ray absorption spectroscopy.

This presentation aims at highlighting approaches and developing ideas on the adaptation of photoelectron, X-ray absorption and vibrational spectroscopy in electrochemical studies ^[1].

[1] ChemElectroChem 1427 2 (2015)

Photoemission spectroscopy for understanding the energetics of thin-film photovoltaic devices

Antoine Kahn

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The quantitative determination of the electronic structure of all materials and interfaces comprised in thin film photovoltaic cells is of paramount importance for understanding charge carrier creation and collection mechanisms and for optimizing device performance. UV to X-ray photoemission spectroscopy is a key tool for achieving this goal, and this talk illustrates this point with three examples. The first pertains to the relation between the “photovoltaic gap” in the active layer of organic single heterojunction or bulk heterojunction solar cells and the open circuit voltage produced by these devices ^[1-3]. The second refers to the choice of carrier selective interlayers in hybrid organic inorganic perovskite solar cells ^[4,5]. The third looks at the low temperature formation of a hole-blocking TiO₂ ultra-thin layer that preserves the integrity of a H-terminated Si surface in a silicon solar cell ^[6,7]. In each case, direct (and inverse) photoemission spectroscopy is used to determine energy level alignment and interface chemistry that are critical to these devices. The advantage that synchrotron radiation photoemission would bring to this important class of studies is clearly pointed out.

References:

- [1] Rand et al., Phys. Rev. B **75**, 115327 (2007)
 - [2] Guan et al., Org. Electr. **11**, 1779 (2010)
 - [3] Wilke et al., Appl. Phys. Lett. **101**, 233301 (2012)
 - [4] Schulz et al., Energ. & Envir. Sci. **7**, 1377 (2014)
 - [5] Schulz et al., Adv. Mat. Int. **2**, 1400532 (2015)
 - [6] Avasthi et al., Appl. Phys. Lett. **102**, 203901 (2013)
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Studying the nature of de defects in various silicon materials used in photovoltaic applications.

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Monocrystalline (c-Si), multi-crystalline (mc-Si), hydrogenated amorphous silicon (a-Si:H) and nano-crystalline silicon (nc-Si:H) are silicon materials that are used in a variety of photovoltaic device configurations. The defects in these materials can limit the performance of solar cells due to Shockley-Read-Hall recombination. The a-Si:H material is used in thin film silicon (TF-Si) devices as absorber layer and as passivating junction layers in c-Si heterojunction (c-Si HJ) solar cells. The electrical quality of a-Si:H suffers from the Staebler-Wronski effect (SWE) which is the creation of metastable light induced defects (LIDs) during light soaking. In this contribution we report on a wide variety of analytical approaches to study the nature of the LIDs.

First, the structural and electrical properties of metastable defects in various types of a-Si:H have been studied using a powerful combination of continuous wave electron-paramagnetic resonance spectroscopy, electron spin echo (ESE) decay measurements, and Doppler broadening positron annihilation spectroscopy. The observed dependence of the paramagnetic defect density on the Doppler S parameter indicates that porous, nanosized void-rich materials exhibit higher spin densities, while dense, divacancy-dominated materials show smaller spin densities. However, after light soaking more similar spin densities are observed, indicating a long-term defect creation process in the SWE that does not depend on the a-Si:H nanostructure. From ESE decays it appears that there are fast and slowly relaxing defect types, which are linked to various defect configurations in small and large open volume deficiencies. A nanoscopic model for the creation of light-induced defects in the a-Si:H nanostructure is proposed.

Secondly, the properties of the a-Si:H/c-Si heterojunction interface are studied by monitoring the passivation quality when samples are exposed to light. The results show that c-Si wafers passivated with a-Si:H may exhibit, not only light induced degradation of passivation quality, but also light induced improvements. In the case of p-type wafers, this light induced improvement is linked to oxide left over before a-Si:H deposition. In the case of n-type wafers it is linked to voids in the microstructure of the a-Si:H. A model to simulate the carrier injection dependent lifetime of c-Si passivated with a-Si:H at elevated temperatures is proposed. Two existing models to respectively calculate the bulk lifetime and surface lifetime are used though these models are currently only presented in literature at room temperature. With this new temperature dependent model in place, in-situ annealing experiments are possible to better analyze the evolution of the passivation quality of a-Si:H.

Correlation of conductivity and electronic structure in metal oxide electrodes and electrolytes: valence band and ligand spectroscopy with x-ray absorption and photoemission

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It is now possible to understand, or at least follow the electric conductivity of metal oxide electrolytes and electrodes on the basis of their x-ray and photoelectron spectra when they reflect the valence band properties. A first example is the quantitative assessment of hole states in solid oxide fuel cell (SOFC) cathodes (polaron conductors), where the relative spectral weight of hole states from oxygen NEXAFS spectra scales exponentially with the conductivity ^[1]. High temperature studies show how this spectral weight changes against the polaron activation energy ^[2]. With the same method we detect *operando* hole states in photoelectrodes when their water oxidation photocurrent sets on ^[3]. In sodium battery cathodes we follow the conductivity and activation energy using oxygen spectra ^[4,5]. Peculiarities in the T-dependent conductivity characteristics of bulk and thin film electrodes are reflected by the same peculiarities in their valence band photoemission and resonant photoemission spectra ^[6-9]. Even ionic transport in ceramic proton conductors can be monitored in analogous way with ambient pressure resonant VB NAP-XPS and impedance spectroscopy ^[10]. Finally I will present an *operando* bio-experiment where an algal biofilm on a photoelectrode is subject to resonant VB PES under water humidity (NAP-XPS), while under complete photoelectrophysiological control and conditions ^[11]. In summary, with precise quantitative analysis of the x-ray/e⁻ spectra it is in general possible to arrive at the correct electric and ionic transport properties, as determined with electroanalytical methods. This approach closes the gap between these two important yet different classes of materials assessment techniques.

References:

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 - [11] A. Braun et al. Chem. Eur. J. 2015, 21(11), 4188-4199.
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In-situ Studies of Oxidation and Hydrogenation Catalysts

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Chemical conversion of low-value reactants into fuel or other added-value products plays an important part in energy scenarios for the future. Catalytic hydrogenation and oxidation reactions are amongst the most important classes of reactions in this context. I will present examples of in-situ XPS and NEXAFS studies of such reactions ranging from single-crystal model catalysts (for hydrogenation of organic molecules) to industrial supported catalysts (for methane oxidation). Surface-sensitive electron-based in-situ experiments of heterogeneous catalysts are limited by the attenuation of X-rays and electrons in the reaction environment, charging and high levels of dispersion of catalyst material. The results show how the catalyst surface and the surface species are affected by ambient gas or liquids.

Abstracts of the Magnetism Session

Monday, 7th of December

Location: "Kino" Building 13.10

Terahertz-to-Infrared Spectroscopy in High Magnetic Fields: Application to Molecular Magnetic Materials

Stephen Hill

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The US National High Magnetic Field Laboratory (NHMFL) recently carried out a series of strategic planning exercises (including several international workshops) focused on the scientific opportunities that would be realized by locating a high-intensity terahertz-to-infrared light source alongside a high magnetic field facility. The first part of this presentation will summarize opportunities in which photons are resonant with the energy- and time-scales typically encountered in materials research at high magnetic fields.

The remainder of the talk will focus on research into Molecular Magnetic Materials, a field that has witnessed remarkable progress in recent years. One of the key ingredients for designing technologically useful molecular building blocks is the magnetic anisotropy that can give rise, e.g., to magnetic bistability in nanoscale memory devices. This anisotropy manifests as large zero-magnetic-field energy gaps between quantized angular momentum projection states. As researchers explore increasingly anisotropic molecular materials, the need for intense tunable photon sources spanning the full terahertz-to-infrared range becomes more urgent ^[1]. Importantly, such sources should be combined with high-field magnets with optical access in order to disentangle weak magnetic excitations from intense vibrational modes that occur in the same frequency range. Examples of current efforts at the NHMFL will be presented, as well as future prospects at major light sources such as BESSY.

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Exploring surface-adsorbed rare-earth metal-organic molecules by soft x rays

Wolfgang Kuch

Institut für Experimentalphysik, Freie Universität Berlin

Organic molecules as building blocks of surface-mounted nanoscale systems have reached tremendous impact in solid-state physics because they provide both reproducibility as well as structural control on the atomic level by the chemical design of the molecules. Molecules containing rare-earth metal ions are promising candidates for the realization of a surface-mounted molecular spintronics due to their slow relaxation of magnetization. Soft x rays allow the element-specific investigation of such systems. X-ray magnetic circular dichroism (XMCD) in x-ray absorption allows to separately study the magnetic moments of the molecules irrespective of the much higher moment of a ferromagnetic substrate below, with sensitivity to coverages in the dilute submonolayer regime.

I will present two examples of adsorbed rare-earth metal-organic molecules. Endohedral fullerenes can encage three Gd ions while the carbon cage isolates the encapsulated magnetic atoms from aggressive environments. Nevertheless, the molecular magnetic moments can still be controlled across the carbon cage. XMCD measurements reveal that competing ferromagnetic and antiferromagnetic interactions with a ferromagnetic Ni substrate lead to a peculiar temperature dependence of the Gd moments inside the fullerenes [1].

Adsorption of single-ion gadolinium and dysprosium metal-organic complexes on Au(111) causes a distortion of the molecules, evidenced by scanning tunneling microscopy and the polarization dependence of x-ray absorption spectroscopy. In the case of Dy, this leads to a huge anisotropy barrier, while for Gd with its half-filled $4f$ shell no significant anisotropy is induced.

Results were obtained in collaboration with C. F. Hermanns, M. Bernien, P. Stoll, D. Rolf, F. Nickel, Q. Xu, A. Krüger, C. Schmidt, C. Hartmann, T. R. Umbach, J. Kopprasch, J. N. Ladenthin, S. T. Waßerroth, G. Ahmadi, M. Schneider, B. W. Heinrich, C. Czekelius, P. W. Brouwer, E. Schierle, E. Weschke, and K. J. Franke.

References:

[1] C. F. Hermanns *et al.*, PRL, 111, 167203, (2013).

Exploring dynamical magnetism on a fs time-scale ...

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The study of ultrafast dynamics in magnetic materials provides rich opportunities for greater fundamental understanding of correlated phenomena in solid-state matter, because many of the basic microscopic mechanisms involved are as-yet unclear and are still being uncovered. In this research area, new developments in laser-based femtosecond x-ray and extreme-ultraviolet sources make it possible to probe element-specific spin dynamics in multispecies magnetic systems ^[1,2]. These nascent optical tools therefore provide new and detailed information that is mostly not accessible by using visible light, and allow for the design of experiments that can help to identify the microscopic mechanisms of ultrafast spin dynamics ^[3,4]. Using femtosecond soft X-ray pulses we were able to investigate the breakdown of the magnetic coupling in heterogeneous magnetic materials on ultrafast timescales ^[5]. The review concludes with a summary and an outlook to the feasibility of laser control of magnetism ^[6].

References:

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 - [4] Phys Rev Lett 110, 197201 (2013)
 - [5] PNAS 109, 4792–4797 (2012)
 - [6] Science 345 (6202), 1337 (2014)
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Magnetism in Heusler Compounds: Materials Design for Spintronics Applications

Julie Karel¹, Ajaya Nayak¹, Olga Mescheriakova¹, Stanislav Chadov¹, Siham Ouardi¹, Adel Kalache¹, Francesca Casoli², Lucia Nasi², Franca Albertini², Ulrich Roessler³, Gerhard Fecher¹, Jürgen Kübler⁴, Stuart Parkin⁵ and Claudia Felser¹

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4 Institute for Condensed Matter Physics, Technical University Darmstadt, Darmstadt, Germany

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Heusler compounds, a remarkable class of highly tunable materials, exhibit a diverse set of materials properties. In particular, they can host a wide variety of useful magnetic behavior such as uniaxial magnetic anisotropy, ferrimagnetism, high spin polarization, low Gilbert damping and non-collinear spin structures; these properties, among numerous others, make this material class attractive for future spintronics applications. This talk will first discuss general rules that can be used to guide design of Mn-based Heusler compounds with tailored magnetic and electronic properties. Then specific examples from our group will be detailed. For instance, compensated ferrimagnets with giant tunable exchange bias can be realized in Mn-Pt-Ga and Mn-Fe-Ga. Examples of half-metallic ferromagnets and materials with strong uniaxial anisotropy (resulting in perpendicular magnetic anisotropy), both of which are relevant for spin valve devices, will be presented. An example of a spin-gapless semiconductor, Mn_2CoAl , will also be shown. In addition, Mn_2RhSn , which exhibits a non-collinear spin structure and is thus a candidate for hosting Skyrmions, will be reviewed. Finally, perspectives for rare-earth free hard magnets in this material class will be discussed. Throughout the talk, soft X-ray spectroscopy and opportunities for future experiments will be highlighted.

Ultrafast spin dynamics of topological spin structures due to spin-orbit effects

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Topological spin structures that emerge due to the Dzyaloshinskii-Moriya interaction (DMI), such as chiral domain walls and skyrmions possess a high stability and are of key importance for magnetic memories and logic devices.

We have investigated in detail the dynamics of domain walls [1] and we find that in addition to conventional spin transfer torque, also spin orbit torques play a key role [2]. By comparing the wall motion with current-induced magnetization switching in our systems, we can deduce the spin-orbit torques independently of the DMI [2] and we find that the motion observed Ta(5nm)/Co₂₀Fe₆₀B₂₀(1nm)/MgO(2nm) can be attributed to a DMI that is opposite to such stacks with a magnetic CoFe layer pointing to the B at the interface that governs the sign of the DMI [2].

For skyrmions we demonstrate for the first time that we can move a train of skyrmions in a “racetrack”-type device due to spin-orbit torques reliably [3] and we find skyrmion lattices at room temperature in confined geometries [3]. Single skyrmion dynamics is imaged using x-ray holography and from the trajectories a large mass is deduced that directly results from the topology of the skyrmion [4].

Finally we probe the fundamentals of spin-dependent transport in a multilayer structure with THz spectroscopy and directly determine the spin-dependent electron momentum scattering times on the fs timescale [5]. In particular we find, that the conventional GMR measurement technique significantly underestimates the spin asymmetry in the electron scattering.

References:

[1] O. Boulle et al., Mater. Sci. Eng. R 72, 159 (2011).

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[5] Z. Jin et al., Nature Phys. 11, 761 (2015)

Advanced spin-resolved momentum microscopy

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A fundamental concept in solid state physics is the description of electrons in a band structure of independent quasi particles. Of particular importance is the spin of the electron, that gives rise to phenomena like ferromagnetism, spin-polarized surface states, and the discovery of new material classes, like topological insulators.

On the experimental side, the novel concept of momentum microscopy evolved to provide an intuitive and comprehensive insight to these band structures. A momentum microscope captures the complete 2π solid angle of emitted photoelectrons into a high resolution image of electronic states in reciprocal space [1]. With the introduction of imaging spin analyzers, based on the mirror-like reflection of photoelectrons at a tungsten - or more recently, gold passivated iridium [2] - surface, the efficiency of spin-resolved measurements experienced a tremendous boost.

Together with modern synchrotron radiation sources, delivering photon energies from UV to soft X-rays, the electron spin now becomes routinely accessible in photoemission experiments. Here, we discuss examples and prospects, ranging from the tomographic imaging of the spin-resolved Fermi surface of ferromagnets to the rapid band-structure mapping of novel materials.

References:

[1] C. Tusche, A. Krasnyuk, J. Kirschner: Ultramicroscopy (2015), DOI:
10.1016/j.ultramic.2015.03.020

[2] D. Vasilyev, C. Tusche, F. Giebels, H. Gollisch, R. Feder, J. Kirschner: J. Electron Spectrosc. Relat. Phenom. 199, p.10 (2015)

Abstracts of the Spintronics Session

Tuesday, 8th of December

Location: BESSY II Lecture hall

Spin-filtered ToF momentum microscopy: 4D-mapping of k-space objects with utmost efficiency

Gerd Schönhense

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Momentum microscopy has recently set impressive benchmarks, in particular in combination with an imaging spin filter (see talk of C. Tusche). Here we report on a novel approach ^[1] based on time-of-flight parallel energy detection instead of dispersive analyzers. A fast delay-line detector (>5 Mcps, 150ps resolution) provides 3D data recording. The ToF approach is advantageous for synchrotron excitation, in particular for time-resolved pump-probe experiments. The spin-filtered mode was explored at BESSY II (U125-2 NIM) yielding (E_B, k_x, k_y) spin textures with more than 10^4 data points simultaneously. This was shown for surface and bulk Rashba bands of the topological ferroelectric GeTe(111) ^[2] and linear-dispersing anomalous surface states on W(110) ^[3]. In the soft-X range (PETRA III, P04) we observed sharp 3D band patterns up to $h\nu=1300\text{eV}$ at $T=30\text{K}$, with 10^5 - 10^6 data voxels simultaneously (100 k-discs with thickness 30meV and dia. 3\AA^{-1} , best resol. 0.02\AA^{-1}). 4D datasets $I(E_B, k_x, k_y, k_z)$ were acquired with utmost speed. Rapid spin-resolved mapping of the full 3D Fermi surface has a high potential in spintronics and for the observation of ultrafast phenomena. Strategies to utilize multibunch modes are discussed.

References:

- [1] Schoenhense et al., JESRP 200 (2015) 94 ;
 - [2] Elmers et al., arXiv;
 - [3] Kutnyakhov et al., arXiv
-

Toward ultrafast ARPES with soft X-rays

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Time- and angle-resolved photoelectron spectroscopy (trARPES) with femtosecond time resolution is a powerful tool providing direct access to the momentum-dependent electronic structure dynamics near the chemical potential on the time scales of elementary electronic and lattice processes. This direct dynamical information is particularly useful in complex materials where the couplings between various electronic and lattice degrees of freedom determine ground and excited state properties. Temporal discrimination can for example be used to identify the dominant couplings and gain insight into the nature of these couplings.

In practice, however, trARPES experiments are currently limited to photon energies well below 100 eV and they typically lack tunability of the photon energy and pulse duration. The ability to exploit tunable soft X-ray pulses with sub-picosecond to few-picosecond durations would clearly take trARPES to a new level.

Here, I will first give a selective overview of recent femtosecond time-resolved photoemission experiments using high-harmonic-generation and free-electron-laser sources and then try to present ideas on future trARPES experiments at a synchrotron radiation source that can deliver tunable picosecond soft X-ray pulses. The resulting requirements on the photon sources and photoelectron detection system will be discussed.

References:

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 - [3] Faraday Discuss. **171**, 243 (2014)
 - [4] Phys. Rev. Lett. **112**, 207001 (2014)
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First Results and Future Plans of the MAESTRO Beamline at the Advanced Light Source

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Angle-resolved photoemission spectroscopy (ARPES) is a premier technique for the determination of the momentum-resolved electronic structure of materials. In complex materials, many-body interactions can renormalize the energy and lifetime of the electronic states, leading sometimes to novel phases of matter. These effects are readily observable using high-resolution ARPES, which has been used intensely in the past couple decades at synchrotrons. These measurements were traditionally confined to *ex situ* grown materials, but more recently, there has been a growing interest in application of ARPES to new technological materials. This means not only turning to lower-dimensional thin films and heterostructures that can only be synthesized in thin film form, but also developing the ability to study ever-smaller samples. By its nature the ARPES technique requires precise atomic surface control and therefore *in situ* film preparation is becoming a must at synchrotrons.

In this talk I will review efforts at the ALS to integrate *in situ* sample preparation with high energy- and spatial-resolution ARPES, in order to meet the future demand in these areas. In particular, I will present some recent results on graphene and related compounds, as well as in oxide surfaces and interfaces. Most recently, we have begun commissioning experiments using the new “MAESTRO” beamline, the Microscopic and Electronic Structure Observatory, which integrates 4 sample preparation chambers and 3 photoemission chambers in a common ultrahigh vacuum envelope served by an automated sample transfer system. Among the novel features are 1) a new “nanoARPES” instrument capable of ARPES down to 50 nm spatial resolution, which we will use to investigate self-organized and patterned materials and 2) energy-filtered PEEM capable of valence band ARPES spectroscopy, in conjunction with full field imaging using valence band contrast. In this talk, I will also discuss medium- and long-term plans for expanding the capabilities, especially in the areas of programmed (combinatorial) growth strategies to improve sample throughput.

Soft X-ray ARPES at Swiss Light Source: Instrumentation and Spectroscopic Potential

V.N. Strocov

Swiss Light Source, Paul Scherrer Institute, Villigen-PSI, Switzerland

Soft-X-ray ARPES (SX-ARPES) in the energy range around 1 keV benefits from enhanced photoelectron escape depth, sharp definition of 3D electron momentum \mathbf{k} , and resonant photoexcitation delivering elemental and chemical state specificity. SX-ARPES instrumentation at Swiss Light Source ^[1] is hosted by the ADRESS beamline delivering soft X-rays in the energy range from 300 to 1600 eV with resolving power $E/\Delta E$ up to 30K. The incident photon flux above 10^{13} photons/s/0.01%BW combined with optimized endstation geometry overpower the dramatic drop of valence band cross-section at high energies and even stretch SX-ARPES to the most photon-hungry cases of buried interfaces and impurities.

I illustrate applications of SX-ARPES to bulk materials with the perovskite $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ where SX-ARPES resolves the full 3D topology of its Fermi surface connected with the magnetoresistance. A "drosophila" of buried interfaces is $\text{LaAlO}_3/\text{SrTiO}_3$. Resolved with resonant photoexcitation of the Ti^{3+} ions, the interface quantum well subbands show peak-dip-hump spectral lineshape manifesting a multiphonon polaronic state fundamentally limiting mobility of the interface electrons and explaining its temperature dependence ^[2]. An example of the impurity systems is the magnetic semiconductor GaMnAs. Resonant Mn $2p$ photoexcitation identifies the ferromagnetic Mn impurity band as well as its energy alignment and hybridization with the host GaAs bands. These diverse applications illustrate the unfolding spectroscopic potential of SX-ARPES ^[3].

References

- [1] V.N. Strocov *et al*, J. Synchrotron Rad. **21** (2014) 32
 - [2] C. Cancellieri *et al*, Nature Comm. (2015, presently available at arXiv:1507.04723)
 - [3] V.N. Strocov *et al*, Synchr. Rad. News **27**, N2 (2014) 31
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Abstracts of the Solution Chemistry Session

Tuesday, 8th of December

Location: "Kino" Building 13.10

Cooperative dynamics of solutions: Why the first picosecond counts

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The cooperative dynamics of liquids and solutions around room temperature is generally dominated by diffusive motions on the pico- to nanosecond timescale, which is readily probed by dielectric spectroscopy in the microwave region.^[1] Shorter timescales down to ~100 fs, i.e. the frequency range of ~0.1-10 THz, are much less investigated. This has to be regretted because in particular for hydrogen-bonding systems and ionic liquids this transition region from inertia-controlled to diffusive motion is important for rationalizing the emergence of solution structure and understanding fast chemical reactions therein. A further reason to grasp the short-time dynamics of liquids is that it provides a far more stringent test for potential models used in computer simulations than the commonly used structural data. Using examples from the literature and our own research this contribution explains why it is necessary to probe the full dynamics of the system by recording the dielectric function from several MHz to ~10 THz. The information accessible with spectroscopy in the Terahertz and far-infrared region will be discussed. It is argued that in order to get this information not only the absorption coefficient should be accurately determined but simultaneously also the refractive index.

References:

[1] Phys. Chem. Chem. Phys., 11, 8984, (2009)

Elucidating the origins of specific ion effects at nanoparticle-electrolyte interfaces

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The structure of the electrical double layer has been debated for well over a century, since it mediates colloidal interactions, regulates surface structure, controls reactivity, sets capacitance and represents the central element of electrochemical supercapacitors. The surface potential of such surfaces generally exceeds the electrokinetic potential, often substantially. Traditionally, a Stern layer of non-specifically adsorbed ions has been invoked to rationalize the difference between these two potentials; however, the inability to directly measure the surface potential of dispersed systems has rendered quantitative measurements of the Stern Layer potential, and other quantities associated with the Outer Helmholtz Plane, impossible. Here we describe our development of X-ray photoelectron spectroscopy (XPS) from a liquid microjet to measure the absolute surface potentials of silica nanoparticles dispersed in aqueous electrolytes. We quantitatively determine the impact of specific cations (Li^+ , Na^+ , K^+ , and Cs^+) in chloride electrolytes on the surface potential, the location of the shear plane and the capacitance of the Stern layer. We find that the magnitude of the surface potential increases linearly with hydrated cation radius. Interpreting our data using the simplest assumptions and most straightforward understanding of Gouy-Chapman-Stern theory reveals a Stern layer (bounded by the Outer Helmholtz Plane) whose thickness corresponds to a single layer of water molecules hydrating the silica surface, plus the radius of the hydrated cation.

X-ray vibrational spectroscopy of liquid water

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2 Synchrotron Radiation Research Organization, The University of Tokyo, Japan

Recent high resolution O 1s resonant inelastic X-ray scattering (RIXS) spectra reveals vibrational energy in the OH-stretching mode^[1]. At pre/post edge excitations the RIXS vibrational energy is blue/red shifted compared to the standard Raman spectra because water molecules with a highly weakened or broken donating hydrogen bond are selected by the pre-edge excitation, while those with tetrahedrally coordinated hydrogen bond are selected by the post-edge excitation. This strongly supports the interpretation of O 1s XAS/XES results of liquid water in terms of a mixture (micro-heterogeneity) model, where the network is considered as a mixture of various hydrogen bond configurations. The 'vibrational RIXS' technique bridges hydrogen bond configuration and the electronic structure of water, which can be applied to a wide range of solutions in the near future.

References:

[1] Phys. Rev. Lett. 111, 193001 (2013).

Atmospherically relevant aqueous surfaces

Olle Björneholm

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Aerosols are major unknowns in climate models, and a better understanding of them is important for improved climate modeling [1-3]. The climate effects of atmospheric aerosol particles are governed by their numbers, sizes, and chemical properties. Particles in the atmosphere are typically mixtures of both organic and inorganic species together with water, see fig.1, and due to their small size, it has become evident that a description using the average bulk composition of an aerosol particle is not enough to describe its climatically relevant properties; a more detailed picture of the surface vs. bulk composition of the aerosols is needed.

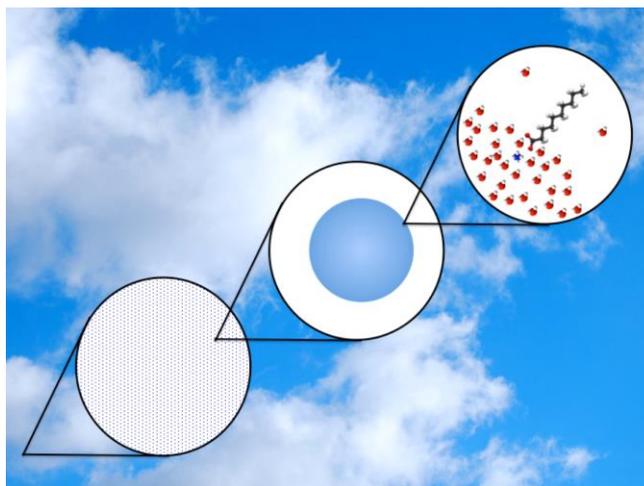


Figure 1. A microscopic view of aerosols.

Progress towards this goal obtained in close collaboration between molecular physicists and atmospheric scientists by XPS on a liquid micro-jet combined with MD will be presented. The influence of environmentally important parameters such as concentration, pH, and ionic strength, on the molecular surface structure of aqueous solutions will be discussed. Examples may include how the microscopic surface composition of succinic acid solutions is connected to macroscopic surface properties [4], how the surface composition of alcohol solutions is affected by chain length, bulk concentration, and isomer effects [5], how surface acid/base chemistry may differ from that of the bulk solution, as well as surface-specific reactions [6,7].

References

- [1] IPCC, 2013: Summary for Policymakers. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [T. F. Stocker et al (eds.)]. Cambridge University Press, Cambridge, UK and New York, NY, USA.
- [2] M Kanakidou et al., Atmospheric Chemistry and Physics 5, 1053 (2005)
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- [5] M-M Walz et al., Phys. Chem. Chem. Phys., accepted for publication
- [6] NL Prisle et al., Atmos. Chem. Phys. Discuss. **12**, 12227 (2012)
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Abstracts of the Correlated Materials Session

Tuesday, 8th of December

Location: BESSY II Lecture hall

Structural and Electronic Dynamics in Transition Metal Dichalcogenides

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3 Paul-Scherrer-Institut, Switzerland.

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Transition metal dichalcogenides (TMDC) are layered crystalline 2D materials with peculiar properties: while a subgroup shows pronounced correlation effects and charge density wave (CDW) formation, others, like Mo and W-based compounds, exhibit pronounced excitonic effects and strong spin-orbit coupling. We investigate ultrafast structural and electronic dynamics in WSe_2 and $TiSe_2$ employing femtosecond electron diffraction (FED) and XUV-based time- and angle-resolved photoelectron spectroscopy (trARPES).

In the CDW material $TiSe_2$, trARPES reveals a pronounced correlation between the backfolded valence band and the structural amplitude mode of the CDW phase. In the semiconductor WSe_2 , we investigate electron relaxation and electron-phonon interaction subsequent to electronic excitation localized in k -space with FED and trARPES.

Finally, we will discuss the development of a 500 kHz XUV source for trARPES. Based on a novel optical parametric chirped pulse amplifier, we achieve a photon flux exceeding 10^{13} photons/s for a high harmonic with 22 eV photon energy. This light source bridges the technology gap between low-repetition rate XUV sources and high-repetition rate UV sources and will provide access to ultrafast excited state electron dynamics in the entire Brillouin zone.

Heterogeneous magnetic order melting launched by ultrafast lattice control at a complex oxide interface

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2 Center for Free Electron Laser Science, 22761 Hamburg, Germany

Transition metal oxides offer a variety of functional electronic properties likely to have a significant impact in applications. In particular, the exceptional sensitivity of these materials to structural distortions paves new ways for the design and control of their phase state, e.g. via strain engineering in oxide heterostructures.

In addition, ultrafast optical control of the lattice as a means to modulate the electronic phases has been demonstrated in these complex oxides. Control of transport and magnetic properties in manganites and light-induced superconductivity in cuprates were demonstrated. These experiments were based on the direct lattice excitation of the bulk, and the photo-excited volume has been driven into the new phase state homogeneously.

Recently, we have extended the same approach to complex oxide heterostructures. By triggering a lattice mode in the LaAlO₃ substrate we drive an ultrafast insulator-to-metal transition in an epitaxial NdNiO₃ film deposited on its surface ^[1].

In my talk, I will show that the spatiotemporal characteristics of this phase transition become accessible by monitoring the ultrafast evolution of the concomitant antiferromagnetic ordering via femtosecond resonant soft X-ray diffraction at the LCLS free electron laser ^[2].

References:

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Direct observation of spin-orbit coupling in iron-based superconductors

Sergey Borisenko¹

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Spin-orbit coupling (SOC) is a fundamental interaction in solids which can induce a broad spectrum of unusual physical properties from topologically non-trivial insulating states to unconventional pairing in superconductors. In iron-based superconductors its role has so far been considered insignificant with the models based on spin- or orbital fluctuations pairing being the most advanced in the field. Using angle-resolved photoemission spectroscopy we directly observe a sizeable spin-orbit splitting in all main families of iron-based superconductors. We demonstrate that its impact on the low-energy electronic structure and details of the Fermi surface topology is much stronger than that of possible nematic ordering. The largest pairing gap is always supported exactly by SOC-induced Fermi surfaces implying a direct relation between this interaction and mechanism of high-temperature superconductivity.

References:

S. Borisenko et al. Nature Physics (in press), arXiv:1409.8669

Search for new f-electron topological materials

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The interplay of strong spin-orbit coupling and electron-electron correlations in f-electron containing intermetallic systems have recently been shown to allow for the emergence of topologically nontrivial surface bands, thereby bringing into existence the new field of "strongly correlated topological insulators". Using a minimum model consisting of localized f-electrons and dispersive conduction electrons with opposite parity, it has been inferred that f-electron systems with cubic and tetragonal symmetries will open both hybridization plus insulating gaps and host topologically protected metallic surface states, if the ground state multiplet is Γ_6 and Γ_8 , respectively [1,2,3,4]. Motivated by this theory, we will present two candidate materials: CeRu₄Sn₆ [5] and SmO [6]. We will discuss the electronic structure of these materials in detail using both synchrotron-based spectroscopic data and parametrized band structure calculations.

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Abstracts of the Life Science Session

Tuesday, 8th of December

Location: "Kino" Building 13.10

From Hard to Soft X-rays: New Insights into Biological Dinitrogen Reduction

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The conversion of dinitrogen to ammonia is a challenging, energy intensive process, which is enabled biologically by the nitrogenase family of enzymes. Both Mo- and V-dependent enzymes are known. However, their activities vary greatly, with the Mo-dependent enzymes being far better at nitrogen reduction, while the V-dependent forms can catalyze C-C bond coupling. Recent work in our group has focused on understanding the electronic structure factors that contribute to these dramatic differences in reactivity. A brief overview of the recent contributions of X-ray spectroscopy to our understanding of biological nitrogen reduction will be given. This will include both high-resolution X-ray spectroscopy in the hard X-ray regime, as well as more recent experiments in the soft X-ray regime (include XMCD and 2p3d RIXS), which promise to further the electronic structural insights that can be obtained.

Surprises in very-high-frequency electron paramagnetic resonance.

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Electron paramagnetic resonance (EPR) is usually carried out at frequencies near 10 GHz. At frequencies above 200 GHz (magnetic fields above 7 Tesla), the physics and technology of EPR changes in ways that are especially exciting for the life sciences. In this frequency range, one can think of EPR as an optics rather than an electronics experiment, the spin polarization can approach 1 at liquid Helium temperatures,^[1] and spin labels based on spin-7/2 Gd³⁺ becomes very attractive.^[2] UC Santa Barbara's MM-wave Free-Electron Laser forms the basis for a unique very-high-frequency EPR spectrometer^[3] that is complementary to other instruments operating in this frequency range.

References:

- [1] Takahashi, S.; Hanson, R.; van Tol, J.; Sherwin, M. S.; Awschalom, D. D., Quenching spin decoherence in diamond through spin bath polarization. *Physical Review Letters* **2008**, *101*, 047601.
 - [2] Edwards, D. T.; Ma, Z. D.; Meade, T. J.; Goldfarb, D.; Han, S. G.; Sherwin, M. S., Extending the distance range accessed with continuous wave EPR with Gd³⁺ spin probes at high magnetic fields. *Physical Chemistry Chemical Physics* **2013**, *15*, 11313-11326.
 - [3] Takahashi, S.; Brunel, L. C.; Edwards, D. T.; van Tol, J.; Ramian, G.; Han, S.; Sherwin, M. S., Pulsed electron paramagnetic resonance spectroscopy powered by a free-electron laser. *Nature* **2012**, *489*, 409-413.
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Toward Molecular Movies of Metalloenzyme Catalysis Using fs X-ray Pulses – Studies on Photosystem II at LCLS

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Biological catalysis of many important products involves the participation of metallo-enzymes. One important example is the large dimeric membrane protein photosystem II (PSII) that catalyzes the light driven oxidation of water into molecular oxygen and protons in all plants, algae and cyanobacteria. The exact reaction mechanism of this thermodynamically challenging transformation is still not known and a detailed knowledge of it could yield important clues to improve artificial catalysts for water oxidation. The recent advances in X-ray sources provided by the development of X-ray lasers (for example the LCLS at Stanford) bring the ultimate goal of recording molecular movies of such molecular machines in action closer to reality. By combining X-ray diffraction and X-ray spectroscopic methods with ultra bright and short (fs) pulses of such an X-ray laser it is possible to extract information from very dilute systems at room temperature before the manifestation of radiation induced changes. We have applied this approach using fs X-ray pulses at the LCLS to study the electronic and geometric structure of the active site of photosystem II, a Mn_4CaO_5 cluster and measured simultaneously oxidation state sensitive X-ray emission and X-ray diffraction data.^[1,2] The results of these studies for several different illumination states of PSII will be presented. In addition we have developed a setup to record transition metal L-edge spectra³ from solutions of metalloenzymes under physiological conditions and applied this to PSII. This allowed us to collect the first partial Mn L-edge spectrum of PSII.

References:

[1] Science,340,491,(2013)

[2] Nature Comm,5,4371,(2014)

[3] J Phys Chem Lett,4,3641(2013)

Time-resolved photoelectron study of excited state dynamics in solution

Franziska Buchner, Hans-Hermann Ritze and Andrea Lübcke

Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany

Time-resolved photoelectron spectroscopy probes the dynamics of photoreactions in time and energy by mapping the excited state into the ionization continuum. Recently, this technique has been advanced by combining it with a liquid microjet allowing to study photoreactions in natural, i. e. aqueous environment. We have applied this technique to obtain new insights into the photoprotection mechanisms of DNA bases and nucleosides. It is well known that DNA bases can very efficiently convert electronic energy into heat by ultrafast internal conversion pathways exploiting conical intersections. Our data show a new relaxation pathway in thymine and provide indication for an additional pathway in cytosine and guanosine. Additionally, in guanosine we suggest the involvement of a doubly-excited state in the photoionization process. I will explain the experimental technique and discuss our observations on the dynamics of photoexcited DNA bases in detail. Furthermore, I will discuss the possible impact of involved doubly-excited states on time-resolved photoelectron spectroscopy.

Poster Abstracts

Monday, 7th of December

BESSY II Foyer

1 Applications of soft and hard X-ray RIXS to ferric model complexes

Anselm W. Hahn, Benjamin van Kuiken, Sergey Peredkov, Dimitrios Manganas and Serena DeBeer

Resonant inelastic scattering (RIXS) has the potential to provide insights into chemical catalysis, by allowing for a direct probe of the metal d-to-d transitions. A longterm goal is the application of RIXS to understanding the process of N₂ reduction. We have started to investigate a series of small molecule model complexes using different types of resonant inelastic scattering (RIXS). The sample set consists of two octahedral low-spin [Fe(Tacn)₂] (Cl₃) and (K₃)[Fe(CN)₆], and has been investigated by 1s3p and 2p3d RIXS. A theoretical description realized by the quantum chemistry program package ORCA, utilizes the Restricted Open-Shell Configuration Interaction with Singles (ROCIS) quantum chemistry methods. Future applications to catalytic systems will be discussed.

2 FTIR spectroscopy view of the proton exchange membrane (PEM) dynamics

Puskar L, Ritter E, Aziz E F, Schade U

Light driven water oxidation is a vital step in harvesting the solar energy, in nature, efficiently performed by photosystem II. Catalysts oxidising water at potentials close to thermodynamic limit are of special interest. The high proton conductivity and stability of ionomer membranes (PEM) makes them popular for catalyst immobilization inside fuel cells. MIR and FIR were applied to investigate the nature of interactions in multi acid side-chain ionomers.

3 In situ Infrared Study of Transition Metal Oxide Water Oxidation Catalysts

Lifei Xi, Christoph Schwanke, Ullrich Schade, Kathrin Aziz-Lange

A new emerging water oxidation catalyst generated via electrodeposition from aqueous solutions containing borate and transition metal ion, eg. Ni and Co, has been studied by in situ infrared absorption spectroscopy coupled with attenuated-total-reflection (ATR). The spectra of water and Ni-or CoBi on ZnSe/Cr/Au electrode surfaces changes in intensity as the potential changes, which are interpreted in terms of the potential-dependent realignment of the water and borate molecules in the film. Two superoxide surface intermediates were observed at high potentials for CoBi film.

4 Monitoring the formation of a CdS / Cu(In,Ga)Se₂ interface

T. Kunze, P. Jackson, D. Hariskos, W. Witte, D. Gerlach, Y. Yamashita, T. Chikyow, S. Ueda, R. Felix, R. G. Wilks, M. Bär

Solar cells based on Cu(In,Ga)Se₂ are considered to be a high-efficient alternative to silicon-wafer based solar cells. In order to monitor the formation of the CdS buffer layer/Cu(In,Ga)Se₂ absorber interface we studied a CdS thickness series. We performed HAXPES measurements at BESSY II (HiKE at KMC-1) and Spring-8 (BL15XU) to analyze how the chemical and electronical

structure changes with increasing CdS thickness.

5 PEAXIS at BESSY II: Design of the new Endstation for RIXS and XPS Measurements and Potential Applications

Ch. Schulz, T. Hofmann, K. Lieutenant, M. Yablonskikh, K. Habicht J. Xiao and E. F. Aziz

We present a new endstation for Photo Electron Analysis and X-ray resonant Inelastic Spectroscopy (PEAXIS) at BESSY II. Its expected performance is shown by means of ray tracing simulations. Additionally, potential applications like element-specific and momentum-resolved studies on elementary (for instance electronic) excitations in thermoelectrics and catalysts for energy conversion are discussed.

6 UPS and XPS investigations of UV/VIS radiation provoked degradation effects of organic thin films

Erik Darlatt, Burhan Muhsin, Roland Rösch, Michael Kolbe, Hendrik Kaser, Alexander Gottwald, Cosmin Lupulescu, Friedrich Roth, Wolfgang Eberhardt, Harald Hoppe, Mathias Richter

A study of radiation induced degradation effects of organic thin films relevant for photovoltaic applications is presented. The irradiation procedure (monochromatic and quantifiable synchrotron radiation exposure in the spectral range from UV to visible light) at the insertion device beamline at the Metrology Light Source is explained. The characterization of the thin films and the investigation of degradation effects were carried out by UPS and XPS measurements before and after radiant exposure.

7 Ferrum: A new highly efficient Spin Detector for Electron Spectroscopy

M. Escher, N.B. Weber, M. Merkel, Focus GmbH, Hünstetten, Germany, M. Johansson, SPECS Surface Nano Analysis GmbH, Berlin, Germany, L. Plucinski, C.M. Schneider, Peter Grünberg Institute PGI-6, Research Centre Jülich, Germany

We present the design of a highly efficient spin-detector based on exchange scattering from an oxidized iron surface. Adaption to various hemispherical or cylindrical analyzers is possible. Using a spin-rotator or multiple detectors all 3 spin components are accessible. The iron film is grown on a W(100) crystal in-situ. We obtain a Sherman-function of 30% and a reflectivity up to 10%. The detector shows no degradation over weeks in UHV. First results of Graphene/Ir(111) and Fe/W(110) are shown.

8 THz-EPR on High Spin Transition Metal Ions: from Proteins to Energy Materials

Joscha Nehr Korn, Karsten Holldack, Joshua Telsler, Robert Bittl, Alexander Schnegg

Spin couplings provide information about functional high spin states in e.g. proteins or synthetic catalytic complexes that may serve as blue prints for future energy production or storage devices. These information are accessible by electron paramagnetic resonance (EPR). Synchrotron-based Frequency Domain Fourier Transform THz-EPR (FD-FT THz-EPR) allows for

mapping of the EPR over a very wide transition energy and field range (3 to 55 cm⁻¹ and -11 T to 11 T, respectively). We recently upgraded the FD-FT THz-EPR configuration, with a quasi-optical bridge. We present experimental improvements and spectral simulations for FD-FT THz-EPR results, obtained on integer and non-integer high spin states in single molecule magnets, catalytic mononuclear transition metal ion complexes and proteins.

9 Unconventional ferrimagnetism in auxetic NiFe₂O₄ in the crossover to the ultrathin-film limit

Hoppe, M., Döring, S., Gorgoi, M., Cramm, S., and Müller, M.

We explore the enhanced magnetic properties of single-crystalline NiFe₂O₄ films from bulk to ultrathin films. We performed a complementing spectroscopic analysis employing bulk- and surface-sensitive photon spectroscopies (HAXPES, XANES, XMCD). Determining the element-specific valencies and coordinations reveals the absence of any cation inversion, as was held responsible for enhanced MS.

10 Enhanced ferrimagnetism in auxetic NiFe₂O₄ in the crossover to the ultrathin-film limit

Michael Hoppe, Sven Döring, Mihaela Gorgoi, Stefan Cramm, and Martina Müller

We explore the electronic and magnetic properties of single-crystalline NiFe₂O₄ films in the crossover from bulk to the ultrathin-film limit. The goal is to uncover impact of the reduced film dimensionality on an enhanced ferrimagnetism. We performed a complementing spectroscopic analysis employing the bulk- and surface-sensitive photon spectroscopy techniques HAXPES, XANES and XMCD. We quantified the element-specific cationic valencies and spatial coordinations and conclude on the absence of a cationic inversion for all NiFe₂O₄ film thicknesses.

11 Ferromagnet - organic semiconductor interface for molecular spin electronic devices

Sayani Majumdar

Organic or hybrid inorganic-organic spintronics is the newly developing branch of spintronics where the advantages of both the large spin polarization of the ferromagnetic metals and half metals and long spin de-coherence lengths of the organic semiconductors are explored. In the present work, we have done structural, magnetic and transport characterization of interfaces comprised of a half-metallic ferromagnet La_{0.67}Sr_{0.33}MnO₃ (LSMO) and two different organic semiconductors namely Co-Pthalocyanine (CoPc) and rubrene.

12 Spatially resolved oscillation modes of spin hall nano-oscillators In oblique magnetic fields

Ahmad Awad Philipp Dürrenfeld Afshin Houshang Ezio Iacocca Mojtaba Ranjbar Randy Dumas Johan Åkerman

The recent demonstration of so called Spin hall Nano-Oscillators (SHNOs)^{1,2} driven by pure spin currents has greatly increased the versatility of spin transfer torque (STT) driven devices. Here we, for the first time, demonstrate SHNO operation in tilted magnetic fields. The electrically detected modes are spatially resolved via u-BLS that permits the observation and the understanding of the excited modes. We show the existence of two different oscillation modes, a self-localised solitonic bullet mode and a field-localized linear mode. Micromagnetic simulations, using Mumax33, shed additional light on both modes and their mutual interplay, including significant mode-hopping between the two.

13 Core-resonant double photoemission from transition metal surfaces

I. Kostanovskiy, F.O. Schumann, Y. Aliaev, Z. Wei, J. Kirschner

We studied the core-resonant double photoemission process from various transition metal surfaces. We excite either the 3d or 4p core level and detect the Auger and the photoelectron pairs with a coincidence spectrometer. We are interested in a transition which leaves two holes in the valence band. We discuss the difference in energy distributions between two cases. The 3d decay can be explained by a sequential emission while the 4p decay proceeds in a single step.

14 THz-feld control of in-plane orbital order

M. Gensch and Simon Wall

15 Iron L-edge XAS and XMCD studies on Fe-S model complexes related to nitrogenase enzyme

Joanna K. Kowalska, Sonny Lee, Thomas Weyhermüller, Oliver Einsle, Edwige Otero, Serena DeBeer

The breaking of nitrogen bonds is an important biological process providing ammonia resources needed for life on earth. Nature performs this process under ambient conditions via nitrogenase enzyme, utilizing a MoFe₇S₉C active center. Our current goal is to determine the oxidation state distribution of iron atoms in this complex cluster. Recent results, towards this assignment based on iron L-edge XAS and XMCD spectroscopic studies on model complexes relevant to this cluster, will be presented.

16 Synchrotron-based Mid-infrared Single-shot Spectrometer

E. Ritter, L. Puskar, K.P. Hofmann, E.F. Aziz, P. Hegemann, U. Schade

A novel infrared 'Single-shot'-spectrometer for measuring irreversible reaction cascades in the μs timescale is shown. In conventional FTIR spectroscopy, this is either limited to ms, or the sample needs to be cyclic so that the same reaction can be triggered multifold. The device is based on a dispersive approach with a focal plane array detector. Together with IR-synchrotron light, the unique optical concept allows a high S/N in single-shot mode. First spectra obtained with a globar proof the aimed design parameters.

17 BESSY VSR - A Variable Pulse Length Storage Ring -

P. Goslawski, M. Ruprecht, M. Ries, G. Wüstefeld on behalf of the BESSY VSR project team

This poster will present the upgrade project BESSY VSR for BESSY II

18 Investigating nanoplasmonics in diamondoid-metal cluster hybrids

T. Zimmermann, A. Knecht, R. Richter, T. Höhne, M. I. S. Röhr, J. Petersen, T. Lau, R. Mitric, T. Möller, T. Rander

Diamondoids show size and shape dependent optical properties. They are interesting as light-emitting materials due to their intrinsic UV fluorescence. However, the fluorescence quantum yield of pristine diamondoids is low. Plasmon resonance effects are known to enhance absorption and emission in metal particles in the nanometer size regime. Combinations of diamondoids and sub-nanometer metal clusters are promising candidates to study such interactions. We present a set-up for the investigation of nanoplasmonics in size-selected diamondoid-metal clusters.

19 Thermal treatment of chromium (III) oxide with carbonates analyzed by far-infrared/THz spectroscopy

Christian Vogel, Jan Stemann, Karsten Holldack, Ryo Sekine, Ewelina Lipiec and Christian Adam

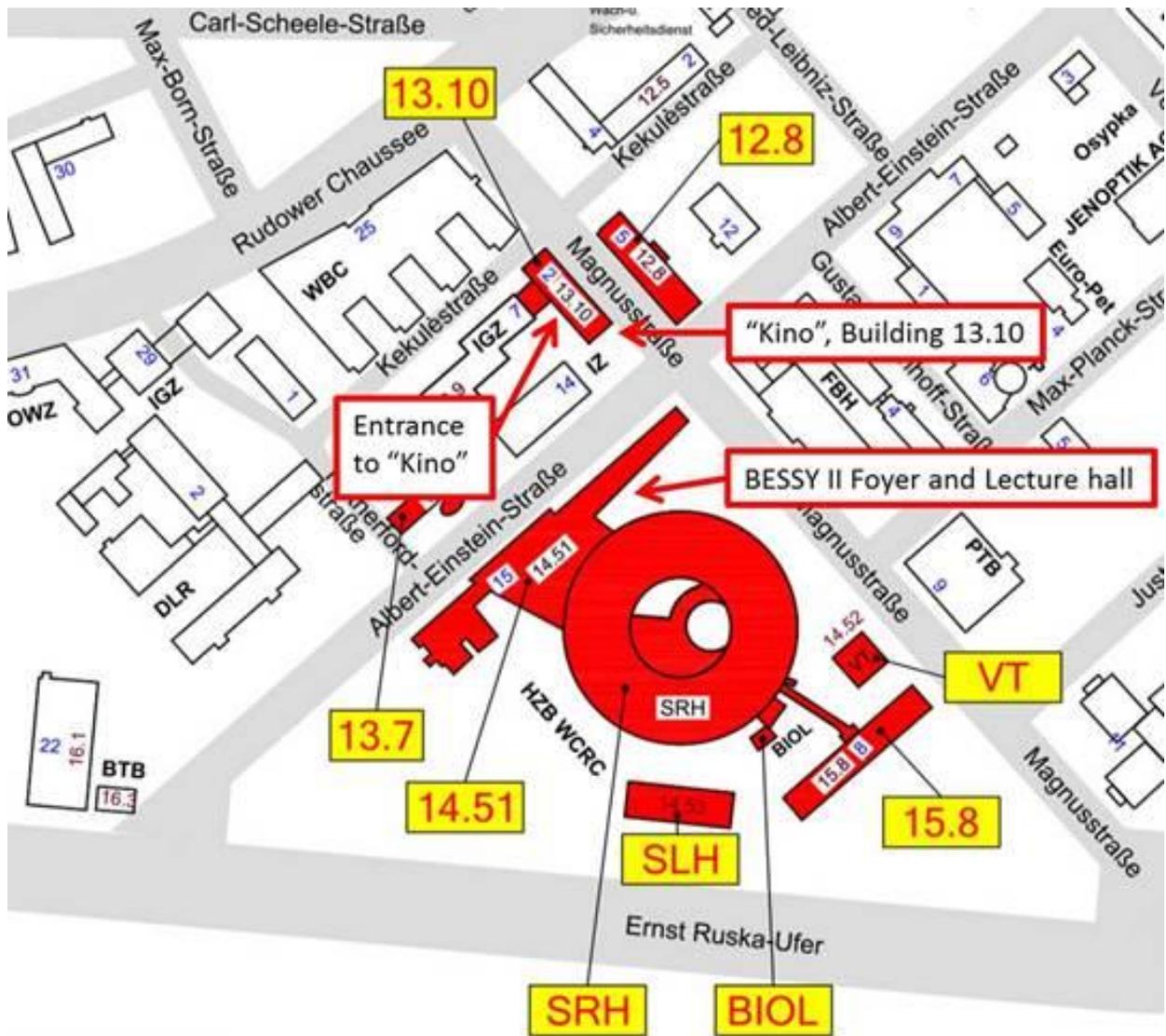
The chemical state of thermochemically treated chromium (III) oxide (Cr_2O_3) with various carbonates was analyzed by far-infrared/THz spectroscopy. Non-toxic Cr_2O_3 was oxidized with potassium, sodium, and calcium carbonate, respectively, to toxic Cr(VI) and Cr(V) compounds during thermal treatment at 1000°C . In reverse, thermochemical treatment of Cr_2O_3 with magnesium carbonate lead to the formation of the Cr(III) compound MgCr_2O_4 . Higher temperatures (1200°C) or reducing atmospheric conditions prevent the formation of Cr(VI)/Cr(V) compounds, too.

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Site plan



Lecture hall:

Overview talks, Sessions Energy Research, Spintronics, Correlated Materials and Into the Future

Kino:

Sessions Magnetism, Solution Chemistry and Life Science

BESSY II Foyer:

Poster Session, Lunch, Snacks

Confirmed Invited Speakers

Martin Aeschlimann (TU Kaiserslautern)
Olle Björneholm (Uppsala Universitet)
Sergey Borisenko (IFW Dresden)
Steven Bradforth (University of Southern California)
Artur Braun (EMPA)
Matthew Brown (ETH Zürich)
Richard Buchner (Universität Regensburg)
Bernd Büchner (IFW Dresden)
Serena de Beer (MPI für Chemische Energiekonversion / Cornell University)
Ralph Ernstorfer (Fritz-Haber-Institut)
Michael Först (Max Planck Institute for the Structure and Dynamics of Matter)
Yoshihisa Harada (University of Tokyo)
Peter Hegemann (Humboldt Universität zu Berlin)
Georg Held (University of Reading / Diamond Light Source)
Stephen Hill (Florida State University / National High Magnetic Field Laboratory)
Antoine Kahn (Princeton University)
Julie Karel (MPI for Chemical Physics of Solids)
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www.helmholtz-berlin.de/user/workshops/thz-soft-x-ray/

