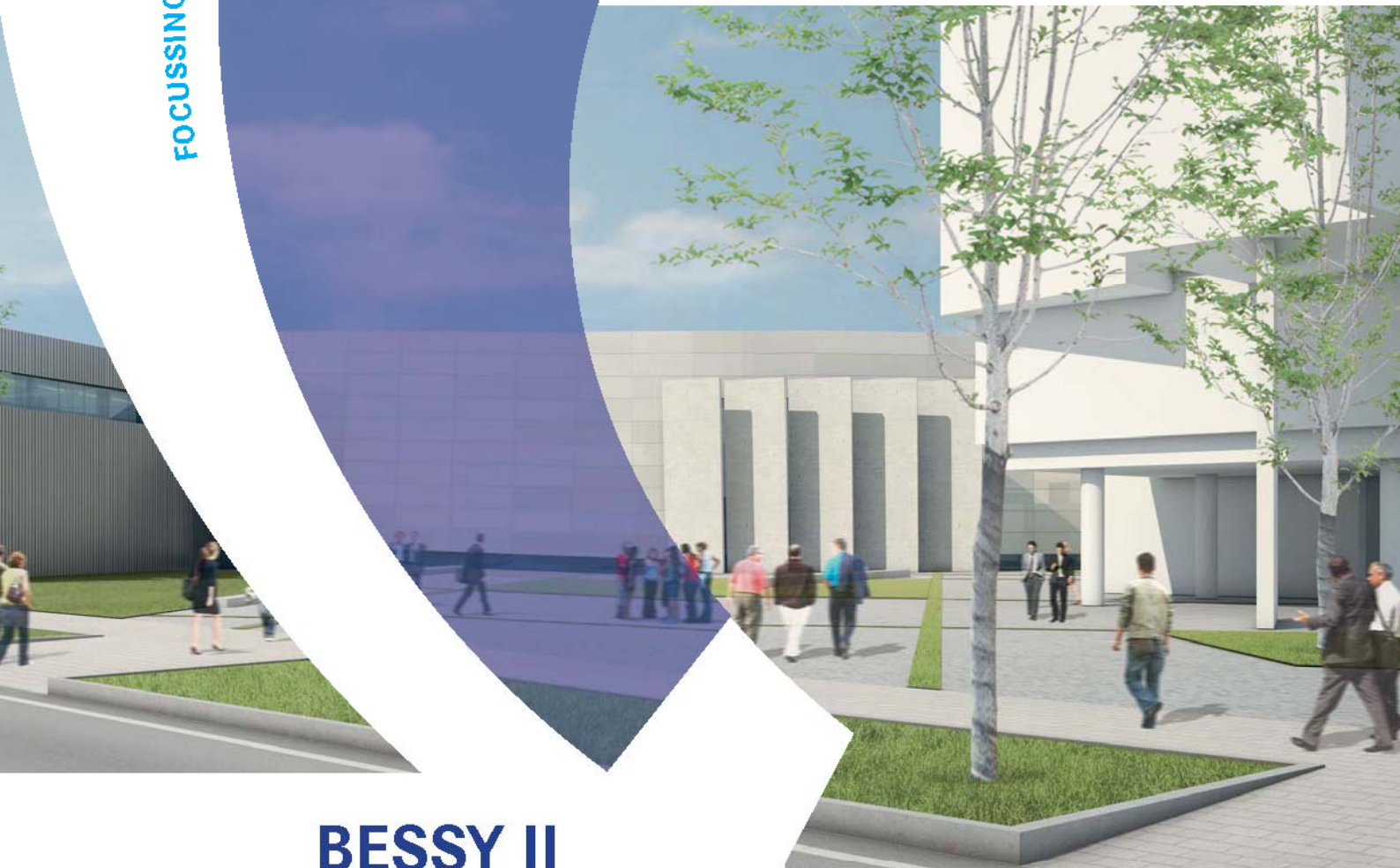


FOCUSSING ENERGY REALIZING VISIONS



BESSY II

FROM PICO TO FEMTO

WORKSHOP ON TIME-RESOLVED STUDIES

January 26 - 27, 2015
Berlin-Adlershof

Dear participant,

HZB kindly welcomes you to our foresight workshop “From Pico to Femto – time resolved studies at BESSY II”.

Already today, the different operation modes at BESSY II (single bunch, low alpha, slicing) enable time resolved studies in the ps to fs regime; they have yielded impressive scientific contributions. Further fostering the investigations on dynamics on a time scale from a few picoseconds to less than 100 femtoseconds with Soft X-rays is at the heart of the BESSY Variable Pulselength Storage Ring (BESSY-VSR) concept. BESSY-VSR is a novel approach to create in the storage ring BESSY II long and short photon pulses simultaneously, which then are available for all beamlines, through a pair of superconducting bunch compression cavities. Proven Pulse-picking schemes will allow each individual user to freely switch between high average flux for X-ray spectroscopy, microscopy and scattering (and thus perform his or her experiment under the same conditions such as photon flux or brilliance as today), and (sub-)picosecond pulses at up to 500 MHz repetition rate for dynamic studies. Indeed, BESSY-VSR preserves the present average brilliance of BESSY II and adds the new capability of user accessible (sub-)picosecond pulses at a high repetition rate. The concept represents the intermediate step towards BESSY III, the successor source for BESSY II. With its unique properties BESSY-VSR offers excellent conditions for making important scientific contributions to socially relevant challenges in areas like energy research (photovoltaics, photosynthesis, catalysis, solar fuels), new quantum materials (nanostructured materials, topological insulators) and information and communication technology (magnetic and optical switches, molecular electronics). We invite you to explore these opportunities with us at the workshop.

The Workshop “From Pico to Femto – time resolved studies at BESSY II” is the second 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,



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

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From PICO to FEMTO

Time resolved studies at BESSY II

(26/27 January 2015)

Topic	Speaker	Affiliation	Time
First Day (Registration BESSY II Foyer)			
Welcome	Alexander Föhlisch		9:15-9:30
Overview Talks (Bessy II Lecture Hall)			9:30-13:00
Magnetism	Theo Rasing	Radboud University	9:30-10:00
Correlated Materials	Steve Johnson	ETH	10:00-10:30
Energy Research/Catalysis	Wilfried Wurth	Universität Hamburg	10:30-11:00
Coffee			11:00-11:30
Bio Systems	Majed Chergui	EPFL	11:30-12:00
Chem. Reaction Dynamics	Kelly Gaffney	PULSE, SLAC	12:00-12:30
Ultrafast from THz to X-ray	Thomas Elsässer	MBI	12:30-13:00
Lunch break (BESSY II Foyer)			13:00-14:00
Topical Sessions: 2 parallel sessions (talks 25 + 5 minutes)			14:00-18:30
Magnetism Location: BESSY II Lecture Hall		Chemical Reaction Dynamics Location: "Kino" building 13.10	
Markus Weigand	MPI for intelligent systems	Christian Bressler	XFEL
Martin Weinelt	FUB	Erik Nibbering	MBI
Claus Schneider	FZJ	Robert Moshhammer	MPI Heidelberg
Uwe Bovensiepen	Universität Duisburg-Essen	Nils Huse	CFEL
Coffee (BESSY II Foyer and Kino)			16:00-16:30
Stefan Eisebitt	TUB	Simone Techert	DESY
Markus Münzenberg	Universität Göttingen	Bernd Abel	IOM, Universität Leipzig
Oksana Chubykalo-Fesenko	CSIC	Oriol Vendrell	CFEL
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment	
Dinner - Poster Session (BESSY II Foyer)			

Second Day (Registration BESSY II Foyer)				
Topical Sessions: 2 parallel sessions (talks 25 + 5 minutes)				9:00-11:40
Energy Research Location: BESSY II Lecture Hall		Bio Systems Location: "Kino" building 13.10		
Thomas Hannappel	TU Ilmenau	Junko Yano	Lawrence Berkeley Nat. Lab	9:00-10:00
Hans-Joachim Lewerenz	Caltech	Tim Saldit	MPI f. Biophysikal. Chemie	
Coffee (BESSY II Foyer and Kino)				10:00-10:20
Rainer Eichberger	HZB	Arwen Pearson	CUI Hamburg	10:20-11:20
Katrin Siefermann	IOM	Thomas Möller	TUB	
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		11:20-11:40
Topical Sessions: 2 parallel sessions (talks 25 + 5 minutes)				11:45-15:05
Correlated materials Location: BESSY II Lecture Hall		Catalysis Location: "Kino" building 13.10		
Michael Foerst	MPI-SD	Jeroen A. van Bokhoven	ETH, PSI	11:45-12:45
Tobias Kampfrath	FHI	Frank de Groot	Utrecht University	
Lunch break (BESSY II Foyer)				12:45-13:45
Matias Bargheer	Universität Potsdam	Martin Wolf	FHI	13:45-14:45
Maurits Haverkort	MPI CPFS	Marcus Lundberg	Uppsala University	
Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		Ideas, Suggestions and Requirements concerning beam, instrumentation and sample environment		14:45-15:05
Coffee (BESSY II Foyer)				15:05-15:30
Into the Future (BESSY II Lecture hall)				
BESSY Accelerator Instrumentation	A. Jankowiak			15:30-16:00
BESSY Photon Science Instrumentation	A. Föhlisch			16:00-16:30
General discussion and Summary				16:30-17:00
End of the workshop 17:00				
Visit of the control room of BESSY II				

Abstracts of the overview talks

Monday, 26th of January

Chair: Claus Schneider

Frank de Groot

Location: BESSY II Lecture hall

Magnetism on the time and length scale of the exchange interaction

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Understanding the physics of magnetism in the regime where the exchange interaction parameters are time-dependent and strongly non-local is a fundamental challenge in modern magnetism. Femtosecond laser techniques have revealed extraordinary responses of the magnetization in many materials that cannot be explained by equilibrium descriptions of magnetism. Various suggestions for explanations include nanoscale non-equilibrium spin dynamics, but experimental data are limited by the spatial resolution of optical laser techniques. In this talk I would like to discuss the challenges in this exciting field and how some of these might be met by the new possibilities of femtosecond X-ray sources. I will present experimental results obtained with the Stanford femtosecond x-ray laser and the Femtoslicing facility of the Helmholtz-Zentrum Berlin that reveal nanoscale chemical and magnetic inhomogeneities and nonlocal transfer of angular momentum between sublattices and nanoregions. An outlook what and how to probe and control magnetic order on the femtosecond time and nanometer length scale and their consequences to engineer new magnetic materials will be discussed.

References:

- A. Kirilyuk, et al, Rev. Mod.Phys. 82, 2731-2784 (2010)
 - I. Radu et al, Nature 472, 205 (2011)
 - J. Mentink et al, Phys.Rev.Lett.108, 057202 (2012)
 - T. Ostler et al, Nature Comm. 3, 666 (2012)
 - A. R. Khorsand et al, Phys.Rev.Lett.108, 127205 (2012)
 - C. Graves et al, Nature Materials 12, 293 (2013)
 - R. Evans et al, Appl.Phys.Lett. 104, 082410 (2014)
 - L. LeGuyader et al, Nature Comm. 2015
-

Using ultrafast x-rays to illuminate pathways for dynamics in strongly correlated materials

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Materials that exhibit strong electronic correlations often exhibit novel and potentially useful properties that either arise directly from these correlations or interact with them in a non-trivial way. These properties include superconductivity, long-range ordering of spin, charge and orbitals, and multiferroicity. In many cases the correlations are driven or at least strongly influenced by strong interactions among multiple subsystems (e.g. spin, charge, lattice).

Here I give a selective overview of recent work on using time-resolved x-ray methods to study such interactions in strongly correlated electron materials. Particular emphasis is given to experiments which illustrate the ability of selective probing offered by x-ray methods to better understand coupling mechanisms that underpin the interesting properties of these materials. Lastly, I give an outlook on the possible applications of the upgraded slicing facility at BESSY II to these problems.

References:

PRL,152,157002 (2014)

Nature,516,71 (2014)

Nature Materials 13, 923 (2014)

PRL,113,026401 (2014)

Science 343,6177 (2014)

Time-resolved studies in catalysis: the quest for transition states

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2 DESY Photon Science, Hamburg, Germany

Energy production and storage with reduced impact on the environment is one of the most important challenges for the coming decades. Heterogeneous catalysis is key to meeting this challenge since nearly all energy conversion processes rely on chemical reactions at solid surfaces. In these reactions the identification of transient intermediates is crucial since they directly indicate which path a reaction is taking, which in turn determines selectivity. The low concentration of such intermediates at any given time in the reaction makes it extremely difficult to observe these intermediates with static experiments. Therefore, the challenge lies in measuring their electronic structure and characterizing them on their ultrashort lifetime of femto- to picoseconds.

New developments in accelerator-based short pulse x-ray sources and lab-based laser technology open up the possibility to directly watch the formation and breaking of bonds and ultimately may enable control on atomic length and time scales.

This work is part of the excellence cluster "Center for Ultrafast Imaging" in Hamburg

References:

M. Dell'Angela et al, Science 339, 1302 (2013)

M. Beye et al, PRL 110, 186101 (2013)

Probing biological function in physiological media by ultrafast X-ray and optical spectroscopy

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Our research focusses on the photoinduced structural dynamics of chemical and biological systems in solutions. For this, we use ultrafast optical and X-ray spectroscopies. X-ray absorption spectroscopy (XAS) reports both on the electronic structure (via the pre-edge bound-bound core transitions) and the geometric ones (via the so-called above-ionization XANES and EXAFS features), which we implemented with picosecond to femtosecond resolution. For the study of biological systems, which have very low concentrations, we have developed a new scheme for optical pump/X-ray probe experiments at MHz acquisition rates. We will present our results on nitrosylmyoglobin (MbNO) in physiological solutions, where we identify the docking site of the NO ligand after photodetachment.^[1]

A full understanding of protein dynamics requires probing the environment, which we do using the naturally occurring amino acids as local reporters. For this purpose, we implemented 2D transient absorption (TA) spectroscopy in the UV below 300 nm, which is where the amino acids (e.g., tryptophan) absorb.^[2] Using 2D UV spectroscopy, we have revealed hitherto unknown electron-transfer processes in haem proteins.^[3,4]

References:

- [1] Element-selective probing of the NO binding kinetics in Myoglobin: A picosecond X-ray absorption study at the Fe K-edge, Mahsa Silatani, Frederico A. Lima, Thomas J. Penfold, Jochen Rittmann, Marco Reinhard, Hannelore Rittmann-Frank, Camelia Borca, Daniel Grolimund, Christopher J. Milne and Majed Chergui, *Nature Chemistry* (submitted)
 - [2] Ultrabroadband femtosecond two-dimensional ultraviolet transient absorption
Gerald Auböck, Cristina Consani, Frank van Mourik and Majed Chergui, *Optics Letters* **37** (2012) 2337
 - [3] Ultrafast Tryptophan-to-Heme Electron Transfer in Myoglobins Revealed by UV 2D Spectroscopy
Cristina Consani, Gerald Auböck, Frank van Mourik, Majed Chergui, *Science* **339** (2013) 1586
 - [4] Tryptophan-to-haem electron transfer in ferrous myoglobins
Roberto Monni, Andre Al Haddad, Frank van Mourik, Gerald Auböck and Majed Chergui
Proceedings of the National Academy of Science (submitted)
-

Understanding Reaction Mechanisms with Orbital and Bond Specificity

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2 PULSE Institute, Stanford University, USA

Understanding chemical reactivity requires the characterization of rare events. The union of ultrafast time resolution with the atomic resolution and specificity of x-ray scattering and spectroscopy present a novel approach to observing chemical reactions experimentally with the atomic resolution needed to construct high fidelity reaction mechanisms and required to test theory and simulation. The value of x-ray methods will be presented in the context of two model chemical reactions: the role of metastable charge and spin distributions in photoelectrochemical reactions and how the reaction environment governs the conversion of photoisomerization and the conversion of photon energy to mechanical and chemical energy.

Ultrafast science – from terahertz to x-ray

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Charge dynamics in the femto- to picosecond time domain play a key role for the electronic and optical properties of solids, for basic chemical and biological processes, and for functional features of new materials. Ultrafast science offers both spectroscopic and structure sensitive methods for the time-resolved observation and analysis of such phenomena and covers a spectral range from the far-infrared to hard x-rays. This talk gives an overview of recent advances in mapping ultrafast charge dynamics in time and space. Strong electric field transients in the terahertz (THz) range are applied to study coherent and dissipative electron transport in solids in a regime of non-perturbative light-matter interactions. Examples are partial Bloch oscillations in semiconductors ^[1] or the novel THz photogalvanic effect in LiNbO₃ ^[2]. Femtosecond x-ray powder diffraction provides transient spatially resolved electron density maps of photoexcited solids as will be illustrated by recent studies of valence electrons in ionic materials ^[3,4].

References:

- [1] W. Kuehn et al., Phys. Rev. Lett. 104, 146602 (2010)
 - [2] C. Somma et al., Phys. Rev. Lett. 112, 146602 (2014)
 - [3] M. Woerner et al., Faraday Disc. 171, 373 (2014)
 - [4] B. Freyer et al., J. Chem. Phys. 138, 144504 (2013)
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Abstracts of the Magnetism Session

Monday, 26th of January

Chair: Maurits Haverkort

Location: BESSY II Lecture hall

Investigating Magnetic Nanostructures using Time Resolved Scanning X-ray Microscopy

M. Weigand¹, I. Bykova¹, M. Bechtel¹, E. Goering¹, H. Stoll¹, B. VanWaeyenberge², G. Schütz¹

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Scanning X-ray microscopy using XMCD as contrast mechanism is a powerful tool to investigate magnetic nanostructures with spatial resolutions even below 15nm. Utilizing the stroboscopic nature of the synchrotron light for pump-and-probe experiments allows the investigation of dynamic phenomena with time resolutions limited by the bunch length of the synchrotron, i.e. below 100 ps.

We will show a variety of experiments performed by users of the MAXYMUS X-ray microscope operated by the MPI-IS at BESSY II, including vortex core dynamics^[1], direct observation of spinwave behavior in film structures and investigations of controlled domain-wall movement in nano-wires^[2,3]. Particular focus will be on the flexibility and efficiency of the method with regard to the individual experiment requirements, utilizing high efficient time resolved experiments in conventional multi-bunch operation

Finally, we will outline how time resolved STXM directly benefits from future developments towards sources with improved bunch timing, i.e. BESSY VSR.

References:

- [1] M. Kammerer et al., Nat Commun **2**:279 (2011)
 - [2] A. Bisig et al., Nat Commun **4**:2328 (2013)
 - [3] J.-S. Kim et al., Nat Commun **5**:3429 (2013)
-

The role of intra- and inter-atomic exchange in the ultrafast magnetization dynamics of Gadolinium metal

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Gadolinium is a prototypical Heisenberg ferromagnet with localized $4f$ magnetic moments. Via intra-atomic exchange the $4f$ moments polarize the $5d6s$ valence-electron spins, which establish ferromagnetic order by inter-atomic exchange. Up to now it was assumed that due to the strong intra-atomic exchange $4f$ and $5d6s$ spin systems show synchronous magnetization dynamics^[1]. However, our recent photoemission studies using high order harmonic generation at 36 eV^[2] show a clear difference in the transients of the $5d$ exchange splitting and the magnetic linear dichroism of the occupied $4f$ states upon laser excitation. This breaking of intra-atomic exchange is well explained by an orbital-resolved Heisenberg model based on *ab initio* exchange parameters^[3].

In line with these results, our recent spin-resolved measurements of the occupied Gd surface state reveal a constant spin polarization for several tens of picoseconds after laser excitation. Again this is surprising because preliminary works lead to the conclusion that the surface state's spin polarization breaks down within the duration of the pump pulse^[4]. Unlike the stable spin polarization, the binding energy of the surface state shifts in accordance with the exchange splitting of the $5d$ bands^[1]. This is in clear contrast to thermal heating where the surface state's spin polarization decreases, while the exchange splitting remains finite even above the Curie temperature.

References:

- [1] M. Wietstruk et al., Phys. Rev. Lett. 106, 127401 (2011)
 - [2] R. Carley et al., Phys. Rev. Lett. 109, 057401 (2012)
 - [3] S. Wienholdt et al., Phys. Rev. B 88, 020406(R) (2013)
 - [4] A. Melnikov et al., Phys. Rev. Lett. 91, 227403 (2003)
-

Studies of Magnetism with XUV Photons from Higher Harmonic Generation

Claus M. Schneider ¹

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Higher harmonic generation (HHG) from noble gas sources provides femtosecond photon pulses with energies up to 100 eV. Since the shallow core levels of the transition metals fall in this regime, HHG enables element-selective investigations of magnetic phenomena in both the static and pump-probe modes with very high time resolution.

We have employed HHG radiation in a variety of photon-in/photon-out and photon-in/electron-out experiments on magnetic systems. Measurements of the transverse magneto-optical effect in reflection revealed the ultrafast demagnetization mechanisms in ferromagnetic alloys and thin film systems^[1]. In the latter, superdiffusive spin currents were shown to contribute significantly to the demagnetization process in a certain excitation regime^[2]. The character of these spin currents can be strongly modified by the choice of the interlayer^[3]. In order to study the magnetic domain distribution in Co/Pt multilayer films and its response to optical excitation we employed resonant magnetic scattering^[4]. In order to directly address the electronic structure of the magnetic systems, we also combined HHG with spin-resolved photoelectron spectroscopy.

References:

- [1] La-O-Vorakiat, C., et al., Phys. Rev. Lett. **103** (2009) 257402.
 - [2] Rudolf, D., et al., Nat Commun., **3** (2012) 1037.
 - [3] Turgut, E., et al., Phys. Rev. Lett. **110** (2013).
 - [4] Weier C., et al., EPL (in print)
-

Femto- and picosecond time-resolved x-ray spectroscopy as an element-specific probe of ultrafast magnetism and lattice dynamics

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Resonant absorption of soft x-rays at $L_{3,2}$ and $M_{5,4}$ edges of transition metals and rare earth elements, respectively, provides local element specific probes which are employed in pump-probe experiments to investigate the response of materials to femtosecond laser excitation. The laser-excited magnetization dynamics in Gd, Tb, and GdTb will be discussed on the basis of pico- and femtosecond time-resolved x-ray circular dichroism using low-alpha and femtosecond slicing at BESSY II combined with table-top magneto-optical experiments. We identify ultrafast magnetic changes with two time scales of 750 ± 250 fs identical for Gd and Tb combined with 40 ± 10 ps for Gd and 8 ± 3 ps for Tb. The faster effect is explained by excitations of the 5d electrons and the slower by spin-lattice coupling of 4f electrons, which is expected to be different for Gd ($L=0$) and Tb ($L=3$) due to their difference in orbital momentum. The element specificity was exploited in an analysis of the GdTb alloy, where a single slower magnetization time scale of 5 ± 2 ps was observed for Gd and Tb, which implies that the slow spin-lattice coupling of Gd is quenched by exchange coupling mediated by the 5d electrons.

Recently, the ultrafast response of Fe-pnictide superconductors to ultrafast laser excitations was analysed at the Fe L_3 edge by time-resolved x-ray reflectivity studies of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$. In picosecond time-resolved studies transient heating effects were found, femtosecond experiments revealed acoustic waves in these materials. As will be discussed, the response of symmetric A_{1g} optical phonons reported for various pump-pump experiments was not observed, which suggests that this resonant soft x-ray experiment probes local changes in symmetry rather than changes of the electronic structure in general.

References:

- M. Wietstruk, A. Melnikov, Ch. Stamm, T. Kachel, N. Pontius, M. Sultan, C. Gahl, M. Weinelt, H. A. Dürr, U. Bovensiepen, Phys. Rev. Lett. **106**, 127401 (2011).
A. Eschenlohr, M. Sultan, A. Melnikov, N. Bergard, J. Wiczorek, T. Kachel, C. Stamm, U. Bovensiepen, Phys. Rev. B **89**, 214423 (2014).
-

Magnetization Dynamics seen via Pump-Probe Holographic X-ray Imaging

S. Eisebitt^{1,2,3}

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2 Gemeinsame Forschergruppe Funktionale Nanomaterialien, Helmholtz Zentrum Berlin

3 Division of Synchrotron Radiation Research, Lund University

Magnetism exhibits phenomena on intrinsic timescales spanning many orders of magnitude, due to its electronic nature including ultrafast phenomena on short length scales. I will demonstrate how x-ray Fourier transform holography (FTH)^[1] can be used in pump-probe schemes to follow magnetization dynamics on the nano-, pico- and femtosecond time scale in real space. Specifically, results on the GHz dynamic behavior of magnetic bubbles (pumped by magnetic field pulses)^[2] and on ultrafast optical demagnetization (pumped by localized IR pulses)^[3] will be discussed. While the first experiment was carried out with ps soft x-ray pulses at BESSY II in single bunch mode, the second was conducted using multiple fs pulses at FERMI. In the light of the different developments of pulsed and coherent XUV/soft x-ray sources, the possibilities in this area of research will be discussed.

References:

- [1] S. Eisebitt et al., *Lensless imaging of magnetic nanostructures by X-ray spectro-holography*, Nature **432**, 885 (2004)
 - [2] F. Büttner et al. *Dynamics and inertia of skyrmionic spin structures*, (Nature Physics, accepted)
 - [3] C. von Korff Schmising et al., *Imaging Ultrafast Demagnetization Dynamics after a Spatially Localized Optical Excitation*, Phys Rev Lett **112**, 217203 (2014)
-

Speed limit of FePt spin dynamics on femtosecond timescales

J. Mendil¹, P. Nieves², T. Santos³, S. Pisana³, J. Nötzold⁴, M. Wolf⁴, M. Battiato⁵, P. Maldonado⁵, P. M. Oppeneer⁵, I. Radu⁶, F. Freimuth⁷, Y. Mokrousov⁷, S. Blügel⁷, U. Martens⁸, V. Zbarsky⁸, J. Walowski⁸, M. von der Eke⁸, O. Chubykalo-Fesenko², T. Kampfrath⁴, M. Münzenberg⁸

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3 San Jose Research Center, HGST, a Western Digital Company, USA

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6 BESSY II, Helmholtz Center Berlin, Germany.

7 Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

8 Department of Physics, Ernst-Moritz-Arndt-University, Germany

Text Magnetization manipulation is an indispensable tool for both basic and applied research. I will demonstrate some of the knobs to tune dynamics at ultrafast time scales. One possibility is to tune shaping the properties of the electronic system. The dynamics of the response depends on the nature of the heat transfer from the laser heated electrons to the spins, which determines the speed of the ultrafast demagnetization. If the electrons are driven to a strong demagnetization, a second slower process is found after the initial fast drop of magnetization, which is a signature of the ferromagnetic correlations. A special material of interest for magnetic hard disc development is FePt. This material has an interesting modification of its density of states: Pt alloying reduces the number of states at the Fermi level and makes the material “more noble”. Consequently, the electron temperatures shoots to much higher values above the Curie temperature. On the other side due to the non-equilibrium electron distribution, also ultrafast currents are generated and contribute to the laser driven spin dynamics. Similarly to shaping the density of states in the first example, adjacent layers of a noble material like Au with sp-states at the Fermi level, or Ru, which has d-band at around the Fermi level, these materials can shape the THz spin currents opening a way towards THz spintronic devices. Here we show first results for more complex devices built up from magnetic tunnel junctions.

References:

J. Mendil, P. C. Nieves, O. Chubykalo-Fesenko, J. Walowski, M. Münzenberg, T. Santos, S. Pisana, arXiv:1306.3112.

U. Atxitia, O. Chubykalo-Fesenko, J. Walowski, A. Mann, and M. Münzenberg, Phys. Rev. B 81 174401 (2010).

T. Kampfrath, M. Battiato, P. Maldonado, G. Eilers, J. Nötzold, S. Mährlein, V. Zbarsky, F. Freimuth, Y. Mokrousov, S. Blügel, M. Wolf, I. Radu, P. M. Oppeneer, M. Münzenberg, Nature Nanotechnology 8, 256 (2013).

Theory for different demagnetization speeds in two-sublattice magnets

Oksana Chubykalo-Fesenko¹, Pablo Nieves¹, Tom Ostler², Roy Chantrell², Unai Atxitia³

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2 University of York, UK

3 University of Konstanz, Germany

The ultrafast excitation of magnetic materials by powerful fs laser pulses leads to magnetisation dynamics on the timescale of exchange interactions. Combined with the XMCD, it allows to access the individual dynamics of different sub-species in the alloy, distinguishable only on this timescale. The unprecedented example of this is the XMCD confirmation of very different dynamics speed of Gd and Fe in GdFeCo alloy, responsible ultimately for its switching^[1]. Simple criteria based on the behavior of one material suggests that the ultra fast demagnetization rate scales as its magnetic moment^[2] or the ratio between magnetic moment and the Curie temperature^[3]. Here we discuss the predictions of the theory based on the Landau-Lifshitz-Bloch equation for two-specie magnets^[4]. We show that the situation there is more complicated and depends on many parameters such as the electronic temperature, inter-sublattice coupling strength, Gd concentration etc. Due to the critical slowing down near the Curie temperature, at high temperatures Fe can become even slower than Gd^[5]. This could allow the control of the polarity of the transient ferromagnetic-like state observed in GdFeCo^[1]. As for the dependence on the Gd concentration, we show that for moderate coupling strength both materials slow down when its concentration increases. For larger coupling, however, the fast material may become faster while the slow one is still slower. This means that in real samples with partial Gd clustering the reversal would start in Gd-rich region, as observed experimentally^[6], while the situation may be reversed if the coupling strength is larger. The conclusions are supported by large-scale atomistic modeling. Finally, we will also discuss ferromagnetically coupled materials, such as permalloy, where we show that in most of situations Ni is faster than Fe.

References:

- [1] I. Radu, et al, *Nature* **472**, 205 (2011)
- [2] N.Kazantseva et al, *Europhys.Lett.* **81**, 27004 (2008)
- [3] B.Koopman et al, *Nat. Mat.* **9**, 259 (2010)
- [4] U.Atxitia et al, *Phys. Rev. B* **86**, 104414, (2012)
- [5] U.Atxitia et al, *Phys. Rev. B* **89**, 224421 (2014)
- [6] C. E. Graves, et. al., *Nat. Mater.* **12**, 293 (2013)

Abstracts of the Chemical Reaction Dynamics Session

Monday, 26th of January

Chair: Kelly Gaffney

Location: "Kino" Building 13.10

Solution Phase Chemistry: Ultrafast Guest-Host and Ligand-Exchange Processes

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In solution-phase photochemistry dynamic solute-solvent interactions can drive the reaction pathway, outcome and efficiency of a chemical reaction. Such interactions involving many-body dynamic processes take place on femtosecond (fs) to picosecond (ps) time scales, and involve simultaneous electronic and structural changes both within the molecule and beyond. Ultrafast x-ray tools sensitive to both the intramolecular electronic (including spin states) and nuclear structural changes including the local solvent structural changes have the potential to disentangle the elementary steps in photochemical reactivity. We present key examples ranging from simple ionic solutes to transition metal (TM) systems studied with the entire arsenal of ultrafast hard x-ray tools (XANES, EXAFS, XES, RIXS, XDS) to unravel the sequence of and interplay occurring during these elementary steps of photochemical reactivity for the first time.

Ligand exchange reactions are key ingredients in biological activity, and occur often at TM reaction centers. We have revisited a model system (aqueous $[\text{Fe}(\text{II})(\text{CN})_6]^{4-}$) to sharpen our x-ray tools, but we also identified a new long-lived reaction intermediate: penta-coordinated $[\text{Fe}(\text{II})(\text{CN})_5]^{3-}$. Both observed 2 ps dynamic (at the SACLA XFEL) and 5 ns kinetic (at APS) processes allow us to generate a picture of the sequence of involved processes.

Finally, future prospects and user opportunities for Chemical Dynamics research exploiting a suite of complementary ultrafast hard X-ray probes at the Femtosecond X-ray Experiments (FXE) instrument of the European XFEL will be presented.

Transient Acid-Base Hydrogen Bond Structure: Probing with IR and with Soft-X-Ray Pulses

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Photoacids are organic aromatic alcohols or protonated amines that exhibit a strong change in acidity (proton donating capability) upon electronic excitation. The pK_a values can be used to predict ultrafast proton transfer rates to accepting bases under aqueous conditions by using Marcus-type relationships that correlate free energy changes and reactivity according to the Förster cycle^[1,2].

The correlation between the O-H stretching frequency and the H-bond distance is well established^[3].

An overview of recent activities on transient IR spectroscopy of hydrogen stretching oscillators of acid-base complexes will be given, with which a direct insight in the structural dynamics of hydrogen bonds of such complexes can be obtained. To disentangle intrinsic charge distribution effects upon hydrogen bond formation from solute-solvent couplings, a joint experimental and theoretical approach based on comparison of transient IR spectroscopy of O-H stretching modes and density functional theory has been applied^[4,5].

To obtain complementary information on the hydrogen bond, soft-x-ray spectroscopy has been shown to be a highly instructive tool^[6]. We have in an initial combined IR and x-ray spectroscopic study investigated the hydrogen bond of N-methylaniline in the polar solvents acetone and DMSO^[7].

The IR spectra support the notion of strengthening the N-H \cdots O hydrogen bond when going from acetone to DMSO. The measured frequency shift of the x-ray absorption pre-edge peak is ascribed to an intricate interplay of transitions from the N 1s to the $N_{LP} \pi^*$ and N-H σ^* anti-bonding orbitals. Future perspectives of time-resolved x-ray spectroscopy of photoacid-base complexes will be discussed. In particular the advance with the implementation of a flatjet system will be made clear.

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Molecular Reactions in Slow-Motion: Experiments with ultra-short XUV Laser Pulses

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Intense ultra-short XUV pulses open new avenues for experiments on the dynamics of atoms and molecules. At present, laser pulses with durations of only a few femtoseconds (5-20 fs) down to the attosecond regime can be produced. The combination of these new sources with many-particle imaging spectrometers (so-called reaction microscopes) for the coincident detection of ions and electrons enable detailed studies at light intensities of 10^{14} W/cm² or more and thus reveal insight into the coupling of light with matter. How does an atom absorb two or more photons from an intense laser pulse, and how is the energy released after the interaction? This and other fundamental processes are subject of ongoing research. Pump-probe experiments with molecules allow the observation of rotational, vibrational and electronic excitations with unprecedented resolution and in real time, and time-resolved experiments with molecules using intense fs XUV Laser pulses are very first steps towards the visualization of fundamental molecular reactions. The general physical and technical concepts will be discussed and recent results will be presented.

Two points of view: transient metal-ligand interactions probed with X-rays

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Bridging the 'time-resolution gap' between X-ray free-electron lasers (XFELs) and synchrotrons holds potential for a lot of transient investigations of solution-phase chemistry and condensed matter such as charge migration, spin transitions, or spatially extended correlated relaxations which often happen on sub-picosecond to few-picosecond timescales. Using high repetition-rate lasers in combination with variable storage rings would allow for many new detailed studies which are hardly feasible at XFELs given the cost and scarcity of experimental opportunities.

I will provide some examples to underscore the prospects of research with variable storage rings for transient X-ray spectroscopy of condensed-phase system, focusing on transition-metal complexes.

Pulsed, High Flux X-ray Sources for Studying Electron Redistribution and Structural Changes in Molecular Switches

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Molecular switches have the potential to be used i.e. in molecular electronics, optoelectronics, in sensor technology or – even – as nano motors in pharmaceutical applications. In order to optimize their performances, ideally the knowledge of their time-dependent structure - function relation is required. Underlying characteristics for all physico chemical transformations or reactions in these systems are bond breaking and bond making processes. Our vision is to optimize these structures towards specific product states by a clever combination of chemical site-specificity, self-assembly and state-selectivity which can be “tuned” from orbital control through the structure of the local environment and selective excitation schemes (heat / optical pulses) to bulk structural changes – or to say it in other words – from the simple to the complex.

In the present contribution we will give an overview on our strategy utilizing the pulsed characteristics of x-ray sources, in particular synchrotrons and free electron lasers, to gain such information for molecular switches in the solid and in the liquid phase. On the x-ray methodological side, molecular crystals form the ideal matrix to proof the capabilities of ultrafast radiation generated with Free Electron Lasers (FLASH at DESY or LCLS at SLAC). In the current contribution we will present our studies on the possibility to collect the “molecular movie” with spatial resolution down to electron density distribution on femtosecond time scales. Last are the typical time scales of atomic and charge movements (in particular within the Born Oppenheimer limit).

Common for all time-resolved x-ray experiments is the applied pump / probe scheme, where an optical pump-laser initiates a reaction whose structural time evolution is then investigated by x-ray probe pulses at various time delays. The x-ray photon-in / photon-out techniques are based on diffraction or spectroscopic techniques like near edge spectroscopy or x-ray emission spectroscopy. Meanwhile x-ray spectroscopic techniques probe the local environment around specific atoms in a molecule - such as orbitals, diffraction studies reveal the structure of the bulk of periodic systems.

Finally, we will present our efforts in systematizing the characteristic structural changes in molecular systems during chemical reactions to some kind of “periodic table” of structural dynamics allowing predicting reaction properties in chemistry from a time-dependent structural point of view.

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Ultrafast EUV Photoelectron Spectroscopy at Liquid Water Microjets

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For decades, ESCA or PES (termed XPS, for X-ray photoelectron spectroscopy, in the case of soft X-ray photons) was restricted to conventional laboratory X-ray sources or beamlines in synchrotron facilities. This approach enabled frequency domain measurements, but with poor time resolution. Indirect access to time-resolved processes in the condensed phase was only achieved if line-widths could be analyzed or if processes could be related to a fast clock, that is, reference processes that are fast enough and are also well understood in the condensed phase. Just recently, the emergence of high harmonic light sources, providing short-wavelength radiation in ultrashort light pulses, added the dimension of time to the classical ESCA or XPS technique and opened the door to (soft) X-ray photoelectron spectroscopy with ultrahigh time resolution. The combination of high harmonic light sources (providing radiation with laser like beam qualities) and liquid microjet technology recently enabled the first liquid interface PES experiments in the IR/UV-pump and extreme ultraviolet-probe (EUVprobe) configuration. In the talk different features of the technology, different promising approaches for high-harmonics generation and a number of recent applications will be highlighted.

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Triggering chemical reactions in solution with strong and short THz pulses

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Pump-probe studies of chemical reactions are almost exclusively limited to photochemistry applications, in which typically a short UV-Vis laser pulse initiates the photoreaction of interest by electronic excitation. In contrast, chemical reactions in the ground electronic state start by random thermal fluctuations of the environment, which supplies the necessary kicks to climb the energy barrier between reactants and products through the transition state.

In this contribution I discuss how the interaction of a strong sub-ps THz pulse with bulk water can result in a T-jump of several hundred Kelvin within one picosecond^[1], and how the transferred energy flows to solute molecules via collisions with the hot solvent^[2].

The ultrafast energy transfer to liquid water can be probed e.g. by x-ray scattering^[1] or an IR probe tuned to the water stretching mode^[2].

Finally, the possible applicability of extreme T-jumps as a way to trigger thermal chemical processes and study their dynamics is analyzed.

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Abstracts of the Energy Research Session

Tuesday, 27th of January

Chair: Marcus Lundberg

Location: BESSY II Lecture hall

Femtosecond transfer studies of photogenerated electrons at (100) interfaces utilizing two-photon photoemission

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Photo-induced electron transfer dynamics is a topical issue of optoelectronics such as photovoltaics or light emitting devices. The ultrafast optical injection of electrons into well-defined, non-equilibrium electronic states of and the subsequent dynamics to reach an equilibrium situation delivers insight into basic transport processes of charge carriers. In particular semiconductors with their well-defined initial equilibrium conditions (occupied and unoccupied bands are separated by an energy gap) are ideal systems for investigating optically induced transport processes via pump-probe experiments. At semiconductor surfaces the transport processes involve states of different character, such as surface (two-dimensional) and bulk (three-dimensional) states, representing an ideal situation in charge carrier transport. Hot electron dynamics at the surface of a semiconductor can be considered a model case for corresponding processes that occur at buried interfaces of electronic devices.

We probed electronic structures of well-defined III-V (100) surface reconstructions with femtosecond two-photon photoemission spectroscopy (2PPE) displaying the ultrafast dynamics of electrons in series of occupied and unoccupied interfacial states and deduced the influence of each particular reconstruction on the electronic structure of the surface ^[1,2]. Photoemission signals arising from bulk optical transitions were distinguished from surface-state related signals by studying the influence of chemical interface modification and by comparing our results to optical in situ measurements (reflectance anisotropy spectroscopy, RAS) ^[3]. These were associated to a broad spectrum of interface analysis methods to obtain a microscopic understanding on the atomic length scale after state-of-the-art preparation via metal-organic vapor phase epitaxy (MOVPE).

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Probing Semiconductor/Electrolyte Interfaces by *Operando* and *In-System* UHV Surface Analyses

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The analysis and optimization of interfaces is crucial for the development of efficient stable light-induced solar fuel generating structures. The advancement from an *in-system* method, where UHV surface analyses after (photo)electrochemical (PEC) conditioning are performed, to an *operando* method for tender X-ray photoelectron spectroscopy (TXPS) is described. Selected experimental results on PEC silicon surface transformations are presented for PEC conditioning in a protective atmosphere followed by direct transfer into UHV. Synchrotron radiation photoelectron spectroscopy (SoLiAs at BESSY) enabled to propose a reaction sequence for the competition between Si dissolution and anodic photooxidation in alkaline electrolyte^[1,2]. As next step in analysis development, an ambient pressure XPS method is described that has been realized at the ALS (Berkeley). First results, performed on a Si-TiO₂ structure that showed exceptional stability as a PEC anode for water photolysis^[3] are presented. Electronic conditions such as depletion layer formation, flatband and Fermi level pinning can be identified using TXPS^[4]. The relevance of reaction dynamics will be outlined for (light-induced) CO₂ reduction where the sequential and the concerted proton-coupled electron transfer occur on different time scales^[5].

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Complementary Time Resolved Studies at Semiconducting Metal Oxides and Quantum Structures for Renewable Energy

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For an advanced development of semiconductor photoelectrodes it is crucial to understand how material composition and preparation parameters are related to carrier transport vs recombination dynamics over a wide time range. For this we investigate bulk and interface reactions of metal oxides such as BiVO_4 , Fe_2O_3 , TaON , TiO_2 and ZnO with time resolved spectroscopy from femtoseconds to milliseconds applying transient absorption, THz and microwave conductivity in transmission and reflection mode. The latter photoconductivity measurements reveal the photo-excited semiconductor carrier lifetime in dependence of (oxygen)vacancies, interstitials, impurities and doping with respect to direct optical band to band excitation or electron transfer from adsorbed molecular sensitizers. Transient absorption supplies information on interfacial electron transfer itself as well as of energetics of bandgap states. THz mobility spectra recorded at different times after photoexcitation yield profiles of the real and imaginary parts of the conductivity that allow for a more microscopic understanding of the transport mechanisms. In addition, two-photon photoemission focuses on surface and surface-near bulk phenomena allowing to monitor the temporal evolution of a photoinduced electron distribution time- as well as energy-resolved within a single experiment. Potentials of this technique will be demonstrated to study electron transfer reactions through transport delaying interface states in hybrid ZnO /organic-dye nanostructures and electron cooling mechanisms in CdSe quantum-well platelet films.

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Dynamics in complex systems revealed by ultrafast spectroscopy with High-Harmonics and X-ray Free Electron Lasers

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Ultrafast dynamics in complex systems, such as in liquid environments or at hybrid interfaces, are of fundamental interest and play an increasingly important role for a variety of emerging technologies. Detailed understanding of ultrafast dynamics in these systems, however, remains a challenge for experiments and theory.

In my talk I will present a new approach to monitor photo-induced electron transfer from a molecule to a semiconductor material with sub-picosecond temporal resolution and from the perspective of well-defined atomic sites^[1]. Combining femtosecond time-resolved X-ray photoelectron spectroscopy with constrained density functional theory, we are able to identify the nature of an intermediate electronic state that precedes free charge carrier generation in a film of dye-sensitized ZnO nanocrystals after photoexcitation of the dye with visible light. The findings demonstrate a new capability to monitor charge transfer in complex hybrid materials.

This presentation will further include picosecond time-resolved photoelectron spectroscopy on liquid microjets. These experiments deliver unprecedented insights into the ultrafast expansion dynamics of supercritical water^[2], or on the nature of dissolved species (e.g. solvated electrons^[3]). In these experiments, the liquid sample is excited with a suitable pump-pulse (IR, VIS, or UV) and probed by recording photoelectron spectra with a probe pulse in the XUV (38.7 eV) obtained via High-Harmonic Generation.

References:

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Abstracts of the Bio Systems Session

Tuesday, 27th of January

Chair: Majed Chergui

Location: "Kino" Building 13.10

Water Oxidation in Natural Photosynthesis

Junko Yano¹

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Photosynthetic water oxidation proceeds through four oxidation steps operating in a cyclic fashion resulting from the successive absorption of four photons by the Photosystem II (PSII) reaction center. The reaction takes place at the Mn₄CaO₅ cluster in the oxygen-evolving complex (OEC) of PSII. The femtosecond X-ray pulses of the free-electron laser make it possible to outrun X-ray-induced damage, allowing studies at room temperature using crystallography and X-ray spectroscopy techniques.

Collective dynamics of membranes by time-resolved x-ray diffraction and coherent imaging

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High spatial and temporal resolution is needed to unravel biomolecular assemblies and the collective dynamics characteristic for supra-molecular aggregation states. To this end, elastic x-ray diffraction typically requires averaging over large ensembles, yielding high resolution in reciprocal space, but to date mostly restricted to the thermodynamic limit. Similarly, inelastic scattering (by x-ray and neutrons) can provide temporal resolution, but again mostly restricted to averaged equilibrium dynamics. These classical restrictions dictated by macroscopic averaging volumes and times can now be overcome by the recent availability of high brilliance synchrotron and free electron laser light.

Here we present time resolved experiments on soft matter samples, in particular on lipid membranes, in the pump-probe scheme using synchrotron (ID09/ESRF, P08/PETRAIII) and free electron laser (FLASH) sources, and different excitation schemes (laser, microwaves, acoustic waves)^[1-3]. In addition, we show how the recent progress in coherent x-ray optics can be used to achieve nanoscale resolution also in real space, dramatically reducing the necessary sample volumes. This makes it possible to probe strongly driven systems, where the small excitation volume so far has precluded studies of out of equilibrium dynamics. Nano-focused x-ray beams also make it possible to study inhomogeneous and hierarchical structures, as we will demonstrate with recent examples measured at (P10/PETRAIII).

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- [1] T. Reusch, F. J. R. Schüle, J. D. Nicolas, M. Osterhoff, A. Beerlink, H. J. Krenner, M. Müller, A. Wixforth, and T. Salditt, Collective Lipid Bilayer Dynamics Excited by Surface Acoustic Waves, *Phys. Rev. Lett.* **113**, 118102 (2014)
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A new data collection strategy for time-resolved experiments using the Hadamard transform

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2 Diamond Light Source, UK

3 University of Edinburgh, UK

In order to fully understand the mechanisms of biological processes, time-resolved methodologies that allow us to comprehend how function is linked to changes in molecular structure are required. Time-resolved X-ray crystallography provides a means of directly visualising structural rearrangements associated with function. Although time-resolved crystallography is a powerful tool, due to both instrument availability and stringent sample requirements it has not been widely applied to biomacromolecules. We have developed a new multiplexing data collection methodology using the Hadamard transform to enable time-resolved structural biology on nano-second to millisecond time-scales. I will present a proof-of-principle study with 200 ms time-resolution to demonstrate the applicability of this method to X-ray crystallography.

References:

Nature Methods 11 1131-1134 (2014)

Ultrafast light induced dynamics in nanoparticles

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The interaction of high intensity, short-wavelength, short-pulse radiation with matter is a fundamental problem of current research. Its understanding is essential for virtually all experiments with new superintense X-ray sources, in particular for flash imaging of nm sized particles. Nanoparticles, especially clusters as a form of matter intermediate between atoms and bulk solids are ideal samples to study fundamental light – matter interaction processes. They are finite systems with the density of bulk solids allowing the investigation of inner- and interatomic phenomena.^[1,2,3] Very recently, initial experiments have shown that nm-sized gas phase particles can be imaged by single shot scattering.^[4,5] Upcoming X-ray lasers will allow improving the resolution and going to smaller particles. This will open new fields for the study of nanoparticles, large molecular aggregates and nanometer-scale science. Ultrafast electron and ion dynamics can be studied with nm spatial resolution by means of time-resolved scattering using pump-probe techniques as well as time of flight spectroscopy. Accelerator based free electron lasers with pulse length in the 10-100 femtosecond regime have already provided a wealth of new results^[4,6] (and references within). Recent studies give evidence that a complicated electron dynamics^[6,7] takes place on a timescale of a few fs or even less.

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Abstracts of the Correlated Materials Session

Tuesday, 27th of January

Location: BESSY II Lecture hall

Mode-selective functional control of complex oxides

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Coherent optical excitation of infrared-active lattice vibrations in solids is emerging as a new tool to control the crystal structure of solids directly^[1] and to drive phase transitions dynamically.^[2-5] Particularly in correlated electronic system, where the phase state is determined by the interactions between charges, orbitals, spins and the crystal lattice, these optically driven structural distortions lead to significant rearrangements in the electronic and magnetic properties, opening up many opportunities for new functionalities.

Here, I will show examples of our efforts in exploiting sub-picosecond diffraction techniques (using the LCLS free electron laser) to gain insight into the dynamics of the complex physics at hand. Hard X-ray diffraction has proven to disclose the vibrationally driven nonlinear crystal lattice response, while resonant soft x-ray diffraction allowed for monitoring transient changes in the electronic and/or magnetic order parameters.

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Probing and controlling spin dynamics with terahertz pulses

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Terahertz (THz) electromagnetic radiation is located between the realms of electronics and optics. Sub-picosecond THz pulses are capable of probing and even controlling numerous low-energy excitations such as phonons, excitons or Cooper pairs^[1]. Here, we consider recent experiments showing that THz spectroscopy is also a highly useful and versatile tool in the field of spin-based electronics (spintronics).

First, we use intense THz pulses to manipulate the magnetic order of solids. This goal is achieved directly by driving magnons in antiferromagnetic NiO with THz magnetic fields^[2]. In a more indirect way, we have recently excited optical phonons in ferrimagnetic Y₃Fe₅O₁₂ (YIG) and observed a magnetization quenching on a surprisingly fast time scale of 1 ps. These results reveal resonantly driven phonons as a new pathway to manipulate magnetic order.

Second, to address spin transport, a femtosecond laser pulse is used to inject spin-polarized electrons from a ferromagnetic into a nonmagnetic metal film. The resulting ultrafast spin current is detected through the inverse spin Hall effect that converts the spin flow into a measurable THz pulse. Choosing nonmagnetic layers with different electron mobility allows one to tailor the temporal shape of the spin current^[3].

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Ultrafast X-Ray diffraction experiments on the nonequilibrium dynamics of thin films near phase transitions

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1 Universität Potsdam, Institut für Physik und Astronomie, Germany

2 Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Ultrafast x-ray diffraction experiments yield precise information on the transient inhomogeneous strain in thin films. We focus on datasets recorded on rare earths multilayers at the new XPP-KMC3 beamline at BESSY II with 100 ps time-resolution and at the laser-driven x-ray plasma source in Potsdam with 100 fs time-resolution.

The latter experiments allow measuring the simultaneous inhomogeneous expansion and compression in (anti-)ferromagnetic Dysprosium films, when we heat the conduction band electrons by laser-excitation. Ultrafast contractive stresses occur when the RKKY exchange interaction is disabled by randomizing the conduction electron spins. On the picosecond timescale, expansive stresses report on the heated electron-phonon system.

The excellent stability of the synchrotron radiation allows measuring simultaneously the Debye-Waller factor as a calibrated monitor of the decreasing lattice heat, whereas the relaxation of the contractive stress reports on the re-ordering of the spin-system and the concomitant entropy loss.

In addition, we observe the transport of excitation energy (heat) via electrons and phonons through the multilayer of Yttrium, Dysprosium and Niobium which is substantially slowed down when heat is captured in the spin-excitations of Dysprosium which contribute half of the specific heat of this material. We experimentally distinguish between direct optical excitation of Dysprosium and triggering the dynamics via fast electron-transport across interfaces.

Correlations and dynamics - ab initio methods away from equilibrium

Maurits W. Haverkort¹

¹ Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The theoretical description of excited systems and their time evolution is challenging. Local correlations combined with delocalized, itinerant states lead in many systems to excitons and resonances with multiplets that are not well described by a single Slater determinant. Technical functionality of a system does not only depend on the ground state, but critically on the time evolution of excitations. One thus needs methods that can predict, for example; how optical excited resonances of a solar cell dye evolve into separated charges, how spin excitations couple to phonons and charge excitations in doped high temperature superconductors, or how the different electronic states in a catalyzer evolve during a reaction.

In this talk I will exemplify how our recently developed method merging ideas from quantum chemistry and renormalization group theory can describe the ground-state, excited states as well as the time evolution of excited systems with equal accuracy.

Abstracts of the Catalysis Session

Tuesday, 27th of January

Location: "Kino" Building 13.10

Time-resolved X-ray spectroscopy on catalysts

Jeroen A. van Bokhoven^{1,2}

1 Paul Scherrer Institute, Villigen, Switzerland

2 Institute for Chemical and Bioengineering, ETH Zurich, Switzerland

Catalysis is the enabling technology in the chemical and refinery industries and in energy conversion processes. Because of the need to advance a sustainable society, new processes using non-fossil-based energy and feedstock resources must be developed. The needed catalyst development is greatly helped by the understanding how a catalyst functions. Many different time-scales are relevant to the catalytic process: from seconds to hours, days, and even months in case of catalyst stability, via (sub)second in case of macrokinetics and (sub)nano-second in case of charge-transfer, to femto-second in case of the actual bond-breaking and bond-making processes. X-ray spectroscopy-based methods are very attractive, as they yield the structure of the catalyst under catalytically relevant conditions. X-ray absorption and emission spectroscopy can be applied at all these time-scales, even though large challenges remain. In the presentation, various relevant time scales and new spectroscopic opportunities will be discussed.

Time resolved experiments in catalysis?

Frank de Groot¹

¹ Debye Institute for nanomaterials science, Utrecht University, Netherlands

Time-resolved x-ray spectroscopy experiments are well-developed to probe the time-evolution of laser-excited states. It is possible to perform such experiments with synchrotrons^[1], x-ray FEL's^[2] and laboratory sources^[3]. As yet, most (excitonic) electronic state calculations for such experiments are based on fixed configurations for the initial, intermediate and final states.

A second topic I will discuss is the potential application of time-resolved experiments to track chemical reactions in a catalytic system at work. Using a dispersive monochromator one can in principle measure an x-ray (emission) spectrum momentarily, allowing fs time-resolved spectroscopy. It remains to be seen how one can couple this to chemical reactions on timescales from fs to ns, μ s, ms and seconds. A complication for fast experiments is the realization of a trigger that is not optical or electromagnetic.

A last topic is the dynamics of core excitation and decay processes by using the energy domain instead of the time-domain. For example using x-ray Raman scattering, one can probe the exact lifetime of excited states.

References:

- [1] JPCL 2, 880 (2011)
 - [2] JPCL 4, 3641 (2013)
 - [3] JPCL 4, 3667 (2013)
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Ultrafast Dynamics of Photoinduced Surface Reactions

Martin Wolf¹

¹ Fritz Haber Institute, Dept. of Physical Chemistry, 14195 Berlin, Germany

Chemical reactions occur usually in the electronic ground state, whereby reaction barriers are overcome by thermal activation. Exceptions from this rule are photo-induced or electron stimulated processes, where the activation is mediated by electronic excitation to an excited state which initiates a nuclear motion along the reaction pathway. Examples are photo-chemical processes and chemical reactions induced by electron attachment or charge transfer. A key concept of chemical reaction dynamics relies on the Born-Oppenheimer (BO) approximation whereby electrons are assumed to follow the nuclear motion instantaneously and thus the reaction evolves electronically adiabatically on a BO potential energy surface. Thereby, non-adiabatic coupling effects between the nuclear motion and the electronic degrees of freedom are neglected. However, electronic non-adiabatic processes can occur at metal surfaces where a continuum of electron-hole pair excitations in the metal may lead to a coupling between electronic and nuclear degrees of freedom and a breakdown of the BO approximation. This is relevant for laser-induced surface femtochemistry at molecule-metal interfaces the dynamics of such processes occur on ultrafast (typically femto- to picosecond) timescales.

In this talk, I will briefly introduce the mechanism of surface femtochemistry using the example of oxidation and desorption of CO on Ru(001). Recent experiments performed with time-resolved resonant inelastic x-ray scattering (trRIXS) at the X-ray free electron laser LCLS provide direct insight into the changes of the electronic structure and chemical bonding after fs laser excitation, leading to a pronounced bond weakening and CO desorption or oxidation. Thereby, motions of CO and O on a Ru(0001) surface are excited allowing the reactants to collide and react leading to the appearance of new electronic states in the O K-edge spectrum. These studies provide new insights into dynamics and details of the potential energy landscape. As an outlook I will discuss some parameters for future time-resolved experiments at BESSY II.

Interpreting X-ray Spectra of Transition Metal Systems: The Core RAS method

Rahul Pinjari¹, Mickael Delcey¹, Meiyuan Guo¹, Michael Odelius², Marcus Lundberg¹

1 Department of Chemistry – Ångström laboratory, Uppsala University, Sweden

2 Department of Physics, Stockholm University, AlbaNova University Center, Sweden

The core restricted active space (RAS) method is an *ab-initio* approach that can be used to simulate X-ray spectra, e.g., metal L-edge X-ray Absorption Spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS), of medium-sized molecular systems without any symmetry constraints.^[1,2] It handles orbitally degenerate ground states, accurately describes metal-ligand interactions, and includes both single and multiple excitations. The performance of the core RAS method is comparable to that of the commonly used semi-empirical charge-transfer multiplet model, see Figure 1a.^[3] Quadrupole transitions have recently been implemented to describe X-ray absorption and scattering in the metal K pre edge. A method has also been developed to analyze the simulated X-ray spectra using a chemically intuitive molecular orbital picture, see Figure 1b. One principal advantage of the multiconfigurational core RAS method is that it correctly describes bond breaking and can therefore be used follow the dynamics of a chemical reaction in the excited state.

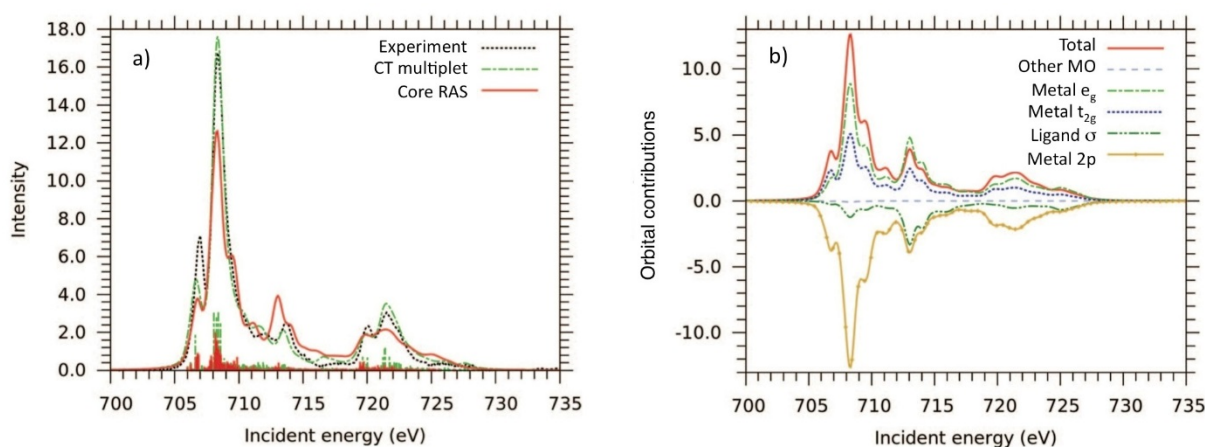


Figure 1. a) Simulations of the metal L-edge XAS spectrum of ferric chloride [FeCl₆]³⁻ using the charge-transfer multiplet model and the core RAS model. b) Analysis of the orbital contributions to the simulated spectrum.

References:

- [1] I. Josefsson et. al., J. Phys. Chem. Lett. 3, 3565 (2012)
- [2] N. Engel et. al., J. Phys. Chem. B 118, 1555 (2014)
- [3] R. Pinjari et. al., J. Chem. Phys., 141, 124116 (2014)

Poster Abstracts

Monday, 26th of January, BESSY II Foyer

1 Recent spectroscopic insights into the electronic structure of FeMo cofactor in nitrogenase

Joanna Kowalska, Ragnar Bjornsson, Frank Neese, Serena DeBeer

Industrially, N₂ reduction requires high temperature and pressure. Nature performs this process under ambient conditions via nitrogenase enzyme, which utilizes the active center - a MoFe₇S₉C cluster. Recent revelation of the central carbide, the assignment of the Mo atom as Mo(III) as well as last XAS and XMCD (both theoretical and experimental) studies of Fe and Mo atoms in model complexes and in the cluster will be presented.

2 Heme regulation of K⁺ channels

Mark Burton, Sofia M. Kapetanaki, Andrew G. Jamieson, Noel W. Davies, John S. Mitcheson, Ralf Schmid, Peter C. Moody, Emma L. Raven, Nina M. Storey

An emerging role of heme is its ability to regulate ion channel function (BK channel, ENaC, Kv1.4). However, the molecular basis of this modulation is unknown. In this work, we have examined heme-dependent regulation in ATP-sensitive K⁺ channels (KATP). We find clear evidence for modulation of cardiac KATP channels by heme and we identify and quantify the heme binding interaction. We use this information to present a broad framework for heme-dependent regulation of ion channels.

3 Fabrication and characterization of thin ceramic layers by sol-gel

El Moussafir El Miloudi

This work concerns Ferroelectrics, whose particularity is to have a variable dielectric permittivity under the effect of a static electric field, should achieve tunable frequency systems without the drawbacks of assets. The use of ferroelectric materials in the solid state, however, was limited until recent years, due to many disadvantages such as high losses. Indeed, the use of ferroelectric films eliminates many problems associated with solid material.

4 Opportunities for time-resolved photoemission experiments on liquids

Unger, I., Förstel, M., Aziz, E. F., Winter, B., Hergenhahn, U.

We have combined a liquid jet with a magnetic bottle spectrometer, which is optimized for electron spectroscopy with synchrotron radiation. We show first results of this set-up and speculate on its use for time domain experiments on the BESSY slicing beamline.

5 Tabletop imaging of the proton migration process in the acetylene cation

Heide Ibrahim, Benji Wales, Samuel Beaulieu, Bruno E. Schmidt, Nicolas Thire, Emmanuel P. Fowe, Éric Bisson, Christoph T. Hebeisen, Vincent Wanie, Mathieu Giguère, Jean-Claude Kieffer, Michael Spanner, Andre D. Bandrauk, Joseph Sanderson, Michael S. Schuurman, François Legare

A pump-(266 nm) probe (800 nm) experiment was designed to follow the isomerisation of acetylene via Coulomb Explosion Imaging. Multi-photon ionization was exploited to overcome high energy barrier and for initiating the dynamics, providing an alternative to technologies such as FEL and High Harmonic Generation based VUV light sources. The experimental results reveal detailed informations and are consistent with ab initio simulations. Ibrahim, Heide, et al., Nature communications 5 (2014)

6 A Quantum Dynamics Study of the Ultrafast Relaxation in a Prototypical Cu(I)-Phenanthroline

G Capano, M Chergui, U Rothlisberger, I Tavernelli, T J Penfold

The ultrafast dynamics of $[\text{Cu}(\text{dmp})_2]^+$ is studied. In agreement with recent experimental conclusions, we find that the system undergoes rapid internal conversion at or near the FC geometry. The flattening of the ligands with a time constant of 400 fs precedes this. Importantly, we show that this latter aspect is in competition with ISC. The mechanism for ISC is dynamic, in that it arises from the system traversing the flattening coordinate where the singlet and triplet states are degenerate.

7 Time-resolved X-ray diffraction study of the piezoelectric deformation of alpha-SiO₂ single crystal induced by a nanosecond electric pulse

Hyeokmin Choe, Semen Gorfman, Michael Ziolkowski, Marco Vogt, Peter Gaal, Ullrich Pietsch

We have studied that (1) the time relation between the longitudinal stress and the generated Rayleigh acoustic waves along the surfaces for the piezoelectric deformation by induced a nanosecond electric pulse and (2) the relationship between the generated strain waves and the inhomogeneous piezoelectric effect (e.g. the change of X-ray diffraction intensity and peak broadening), by probing the dynamics of the X-ray diffraction rocking curve in electrical pumps - X-ray pulse probe technique.

8 THz field control of symmetry-breaking order in correlated materials

Timothy A. Miller, Ravindra W. Chhajlany, Luca Tagliacozza, Bert Green, Sergey Kovalev, Dharmalingam Prabhakaran, Maciej Lewenstein, Michael Gensch, Simon Wall

Nematic, stripe and orbital phases are ubiquitous symmetry-breaking anisotropic ground states in correlated systems such as pnictides, cuprates, nickelates and manganites. Controlling their formation may present new ways to understand the couplings and competition between the phases. Here, we demonstrate that orientation of orbital domains in the manganite $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$ can be controlled, dynamically, by the polarization of an external pulsed THz light field.

9 Structural and Magnetic Dynamics in the Magnetic Shape-Memory Alloy Ni₂MnGa

S.O. Mariager, C. Dornes, J.A. Johnson, A. Ferrer, S. Grübel, T. Huber, A. Caviezel, S.L. Johnson, T. Eichhorn, G. Jakob, H.J. Elmers, P. Beaud, C. Quitmann, G. Ingold

We use tr-XRD and tr-MOKE to measure the laser induced dynamics in a multiferroic MSMA Ni₂MnGa film. We identify a coherent phonon as the amplitude of the modulated structure and an ultrafast phase transition leading to a quenching of the IC structural modulation within 300 fs comparable to the demagnetization time of 320 fs.

10 Ultrafast demagnetization dynamics in TbMnO₃

E. M. Bothschafter, T. Kubacka, L. Rettig, S. Manz, J. Saari, S.M. Koohpayeh, S. S. Dhesi, S. L. Johnson, U. Staub

We present the investigation of demagnetization dynamics in the multiferroic compound TbMnO₃ in a picosecond optical pump- x-ray probe experiment with the goal of establishing how and at which timescales the magnetic order transforms upon resonant photoexcitation. Time-resolved demagnetization dynamics starting from the spin-density wave phase show a comparably slow decrease of the magnetic order within 15 picoseconds and a modification of the magnetic wave vector.

11 Ultrafast structural dynamics of the Fe-pnictide parent compound BaFe₂As₂

L. Rettig, S.O. Mariager, A. Ferrer, S. Grübel, J.A. Johnson, J. Rittmann, T. Wolf, S.L. Johnson, G. Ingold, P. Beaud, U. Staub

We use femtosecond time-resolved x-ray diffraction to investigate the structural dynamics in the Fe-pnictide parent compound BaFe₂As₂, where we observe intensity oscillations of two specific Bragg reflections. Their distinct sensitivity to the pnictogen height demonstrates the coherent excitation of the A_{1g} phonon mode and allows us to quantify the coherent modifications of the Fe-As tetrahedra. In addition, we derive the electron-phonon deformation potential for this particular mode.

12 Time-resolved X-ray diffraction on dysprosium thin films

A.Koc, M.Reinhardt, P.Gaal, W.Leitenberger, M.Bargheer

We use time-resolved X-ray diffraction at the XPP-KMC3 beamline at BESSY II in order to investigate the structural changes and the interactions between electronic, phononic and magnonic degrees of freedom of dysprosium at cryogenic temperatures.

13 Resonant and off-resonant ultrafast demagnetization dynamic in Co₂MnGa Heusler alloy

S. Solopow, A. Kronenberg, L. Le Guyader, T. Kachel, I. Radu, H. Elmers, A. Föhlisch

In a Heusler alloy, the spin dependent density of state shows a band-gap only for one spin direction, i.e. the compound is half-metallic. Here we present results of pump-probe experiments on Heusler Co₂MnGa alloy using circularly-polarized 100 femtosecond long X-ray pulse in reflection geometry to probe the magnetic order. Preliminary experiments with 400 nm and 1200 nm were performed. Different demagnetization time constants for Co and Mn were observed in combination with the pump wave length.

14 Spin wave emission from magnetic vortex cores measured by time-resolved magnetic x-ray microscopy

S. Wintz, V. Tyberkevych, M. Weigand, K. Schultheiss, J. Raabe, J. Lindner, A. Erbe, A. Slavin, J. Fassbender

The investigation of spin wave dynamics in nanomagnetic systems is a key topic of modern magnetism. Here we demonstrate that the excitation of short propagating spin waves is possible in a stacked vortex pair system with opposite circulations and parallel cores. The emitted spin waves ($L \sim 100$ nm) were directly imaged by means of time-resolved scanning transmission x-ray microscopy (Maxymus). The observed frequencies were only limited by the width of the x-ray pulses in multi-bunch mode.

15 Ultra Sensitive Time Resolved X-ray Microscopy at 10 GHz and Beyond using the SSRL STXM

S. Bonetti, H. Ohldag, R. Kukreja, Z. Chen, J. Frisch, H. Dürr, J. Stöhr

In this poster, we illustrate the capabilities of the time-resolved scanning transmission microscope at the Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC. Our instrument is able to measure magnetic moments as small as 0.00001 Bohr magnetons, that allowed us to observe the spins injected into non-magnetic Cu from a Co thin film. Our microscope can also be used to create direct spatial map of magnetization dynamics with 35 nm resolution and at frequencies up to 10 GHz.

16 Laser induced electronic structure modifications and magnetization dynamics in epitaxial FeRh(100) thin films

Dr. F. Pressacco, Prof. Dr. J. Lunning, Dr. V. Uhler, Dr. E. Fullerton, Dr. A. Nicolaou, Dr. M. Gatti, Dr. F. Sirotti

The metallic alloy FeRh undergoes a phase transition from an AntiFerromagnetic to a Ferromagnetic Phase when heated above 400K. We report the time resolved evolution of the electronic structure, with a time resolution of 50 ps, induced by an ultrafast laser pulse (70 fs FWHM). We followed the evolution of the valence band during the demagnetization by measuring the electronic density of state with photon energy of 100 eV and the magnetization dynamics measuring the XMCD contrast of Fe at 709 eV.

17 Unidirectional sub-100-ps magnetic vortex core reversal studied by time-resolved scanning transmission X-ray microscopy

Matthias Noske, Markus Weigand, Georg Dieterle, Ajay Gangwar, Matthias Kammerer, Markus Sproll, Johannes Förster, Hermann Stoll, Manfred Fähnle, Georg Woltersdorf, Christian H. Back, Gisela Schütz

At the MPI MAXYMUS endstation at BESSY II we imaged unidirectional reversal of the magnetic vortex core polarity within less than 100ps. Sub-micron sized Permalloy discs are excited by 45ps long orthogonal magnetic pulses. The application of such short digital pulses is a favourable excitation scheme for technological applications. The movies and experimental phase diagrams obtained for this spin-wave mediated sub-100-ps vortex core switching are in good agreement with micromagnetic simulations.

18 Spin dynamics and ultrafast transport in tunnel-magneto resistance junctions

Jakob Walowski, Ulrike Martens, Marvin von der Ehe, Vladyslav Zbarsky, Markus Münzenberg, Stefan Niehörster, Alexander Böhnke, Karsten Rott, Günter Reiss, Andy Thomas

Excitation of tunnel-magneto resistance junctions by short laser pulses induces spin transport and ultrafast spin dynamics in the magnetic layers. Both effects depend on the magnetic electrodes and the tunnel barrier. We investigate the magneto-Seebeck effect and optimize barriers for thermal spin transfer torque switching. By studying ultrafast dynamics, we want to disentangle the mechanisms causing spin transfer through the barrier on femtosecond time scales.

19 VEKMAG-A new end station at BESSY II for static and dynamic experiments in high magnetic fields

Ryll H, Radu F, Rader O, Noll T, Tennant D A, Chang Y-M, Miguel J, Kuch W, Abrudan R-M, Zabel H, Woltersdorf G, Hollnberger M, Back C.

VEKMAG is a 9T-2T-1T vector superconducting magnet station, which is designed for the time-resolved research of future spintronic materials, such as multi- and single-layer magnetic thin films, nanostructures, and molecules. Experimental probes include XAS, XMCD/XMLD measurements, resonant soft X-ray scattering methods, as well as time-resolved ferromagnetic resonance (FMR) and electron paramagnetic resonance (EPR) using XMCD. The available temperature range extends from 2 K up to 500 K.

20 Spin-orbit driven ultrafast demagnetization in rare-earth alloys

L. Le Guyader, S. Solopow, R. Abrudan, F. Radu, K. Holldack, R. Mitzner, T. Kachel, A. Föhlisch, I. Radu

Understanding the ultrafast demagnetization is a fundamental problem of modern magnetism. Particularly, the spin-orbit coupling LS mediating the spin-lattice interaction is one of the key ingredients. An intriguing case of tunable parallel to anti-parallel LS coupling occurs in rare-earth alloys. Here we report on the properties of such thin films using X-ray Magnetic Circular Dichroism (XMCD). Preliminary femtosecond XMCD time-resolved experiments performed at slicing are presented.

21 Multichannel compact classical 40 kV Mott detector

V.N. Petrov, V.N. Strocov, J.H. Dil

Design of a multichannel electron spin detector based on optical imaging principles and Mott scattering is presented. A multichannel electron image produced by standard angle-resolving electron analyzer by an electrostatic lens at an accelerating voltage of 40 keV onto the Au target. Quasi-elastic electrons bearing spin asymmetry are imaged by magnetic lenses onto position-sensitive electron CCDs. The efficiency gain compared to the single-channel Mott detector can be a factor of 1.5×10^4 .

22 Imaging instantaneous interatomic electron current with ultrafast resonant x-ray scattering

Daria Popova-Gorelova, Robin Santra

We propose ultrafast resonant x-ray scattering (RXS) for imaging dynamical properties of nonstationary electron systems. Employing a rigorous theoretical analysis within the framework of quantum electrodynamics, we demonstrate that a single scattering pattern from a nonstationary electron system encodes the interatomic electron current at the time of measurement. We explain how the instantaneous interatomic electron current can be recovered from a pattern.

23 Coherent ultrafast spin-dynamics probed in three dimensional topological insulators

T. Schumann, F. Boschini, C. Seick, M. Manusrova, G. Mussler, L. Braun, F. Katmis, J. S. Moodera, C. Heiliger, T. Kampfrath, M. Münzenberg

Topological insulators are believed to open up a novel route in spin based electronics. The energy momentum landscape of the Dirac cone provides via spin-momentum locking of the current and the spin a control of the directionality of spin and momentum. Its femtosecond control with light pulses has been demonstrated. Here we demonstrate coherent femtosecond control of spin-polarization and the DC detection of polarization dependent photo currents.

24 High flux table-top water window X-ray source

B. E. Schmidt, N. Thire, S. Fourmeaux, S. Beaulieu, V. Cardin, M. Negro, J-C Kieffer, C. Vozzi, F. Legare

Intense mid-infrared femtosecond laser pulses centered at $1.8 \mu\text{m}$ wavelength, coupled to a new gas cell design, are employed to drive high harmonic generation with high flux down to the soft X-ray regime. We have seen the extension of the cut-off up to 500 eV photon energy with $> 10^7$ photons/second (100 Hz laser) over the water window spectral range. Further scaling of this source to higher repetition rate will be discussed.

25 Ultrafast X-ray Microcalorimeter Spectrometry for Molecular Structure

Jens Uhlig, Joel N. Ullom, William B. Doriese, Ujjwal Mandal, Dharmalingam Kurunthu, Joe W. Fowler, Wilfred K. Fullagar, Fredrik Parnefjord, Dan Swetz, Luis Miaja-Avila, Galen O'Neil, Carl Reintsema, Dan Schmidt, Kevin Silverman, Villy Sundström

We developed a tool for time resolved x-ray absorption and emission spectroscopy by generating a sub-picosecond hard x-ray continuum spectrum from a waterjet plasma using just such a laser system. The novel approach is the use of a single photon measuring cryogenic microcalorimeter array as a high-resolution energy-dispersive detector. With up to 16 kHz laboratory based time resolved x-ray spectroscopy become feasible.

26 Sample Environment for Synchrotron Radiation Experiments

Klemke B, Grimm N, Gerischer S, Wallacher D, Kiefer K

Based on our knowledge and experience in providing sophisticated sample environment (SE) equipment since many years to the neutron users at BER-II reactor, the SE-department at the HZB started additionally to support the synchrotron user at BESSY II. Especially for research areas, where no commercial solutions are available, novel parts of SE equipment have been developed tailored to the needs of the users.

27 Experimental Station A at SwissFEL

Gregor Knopp, Chris Milne, Jakub Szlachetko, Bruce Patterson, Rafael Abela

Free electron lasers are ideal for time-resolved pump-probe and nonlinear X-ray experiments. SwissFEL experimental station A will specialize in applying X-ray spectroscopic and scattering techniques to photochemical and photobiological systems. I will present details of the conceptual design of the experimental station and will cover some recent work we have performed, providing examples of the types of measurements we anticipate will be performed at SwissFEL.

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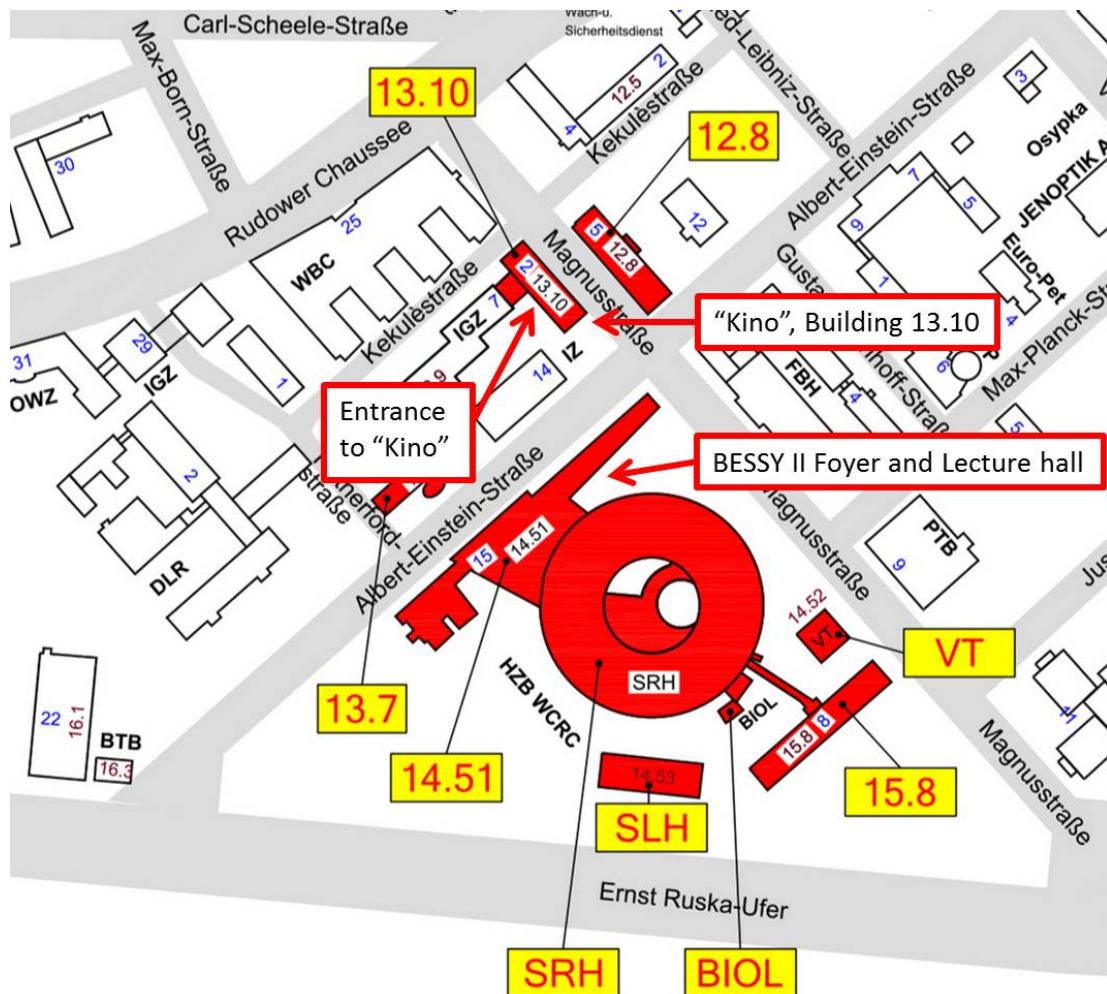
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Site plan



Lecture hall:

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

Kino:

Sessions Chemical Reaction Dynamics, Bio Systems, and Catalysis

BESSY II Foyer:

Poster Session, Lunch, Dinner

Confirmed Invited Speakers

Bernd Abel, IOM, Universität Leipzig
Mathias Bargheer, University of Potsdam
Jeroen A. van Bokhoven, ETH, PSI
Uwe Bovensiepen, Universität Duisburg-Essen
Christian Bressler, XFEL
Majed Chergui, EPFL
Oksana Chubykalo-Fesenko, CSIC
Rainer Eichberger, HZB
Stefan Eisebitt, TU Berlin
Thomas Elsässer, MBI
Alexander Föhlisch, HZB
Kelly Gaffney, SSRL, SLAC
Frank de Groot, Utrecht University
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