Monday, 4 July 2016

Plenary Opening (9:00 – 10:15, Audimax F30)

History, memory and legacy of Wu Ziyu
Mon_Plenary_1
Presented by Augusto Marcelli
This contribution will present the work of Wu Ziyu, Professor and Director of the Institute of High Energy Multidisciplinary Center in Beijing, former Director of the Beijing Synchrotron Radiation Facility (BSRF) of the Institute of High Energy Physics (IHEP) and Professor and Director also of the National Synchrotron Radiation Laboratory (NSRL) of the University of Science and Technology of China (USTC) in Hefei. He won the National Outstanding Youth Fund prize in 2001 and later he was a winner of the Chinese 973 program for chief scientists. His contribution is word recognized as one of the most important for the growth of the Chinese community in synchrotron radiation technology and applications.

Soft and hard x-ray photoemission of buried oxide interfaces
Mon_Plenary_2
Presented by Ralph Claessen
Modern epitaxy methods have made it possible to fabricate heterostructures of complex transition metal oxides with atomically sharp interfaces. Interfacing not only opens new pathways to controlling the electronic and magnetic properties but can also induce novel quantum phases not existing in the bulk of the constituents. Detailed scrutiny of the underlying electronic states requires novel spectroscopic methods with specific interface sensitivity. Photoelectron spectroscopy with soft and hard x-rays is a particularly valuable tool for this purpose, as I will illustrate by our systematic studies of $LaAlO_3/SrTiO_3$ and related oxide heterostructures with their unusual interfacial 2D electron systems.

Session: ARPES 1 (11:00-12:30, Auditorium E3)

Laser ARPES on High Temperature Superconductors
Mon_ARPES1_1
Presented by Xingjiang Zhou
The mechanism of high temperature superconductivity in the copper-based and iron-based superconductors remains a prominent and challenging issue in condensed matter physics. Angle-resolved photoemission spectroscopy (ARPES), as a powerful technique to directly probe the electronic structure of materials, has played a key role in studying high temperature superconductors. In this talk, I will first introduce some latest development of vacuum ultraviolet (VUV) laser-based ARPES techniques. I will then highlight some of our recent results in utilizing the VUV laser-based ARPES to study the copper-based superconductors and the iron-based superconductors.

Isotropic kink in $La_{0.6}Sr_{0.4}MnO_3$ thin films studied by *in situ* angle-resolved photoemission spectroscopy
Mon_ARPES1_2
Presented by Koji Horiba
In order to reveal the many-body interactions in three-dimensional (3D) perovskite manganites, we performed an *in situ* angle-resolved photoemission spectroscopy (ARPES) on $La_{0.6}Sr_{0.4}MnO_3$ and investigated the behavior of quasiparticles. We observed clear kinks throughout the entire hole Fermi surface in the ARPES band dispersion. This isotropic behavior of kinks suggests that polaronic quasiparticles produced by the coupling of electrons with Jahn-Teller phonons play an important role in the ferromagnetic metallic phase of $La_{0.6}Sr_{0.4}MnO_3$.

Ultrafast dehybridization between *f*- and *d*-states in a Heavy-Fermion System
Mon_ARPES1_3

Presented by Dominik Leuenberger
We report evidence for optically induced reduction of the *f-d* hybridization in the prototypical heavy-fermion compound $YbRh_2Si_2$ on a femtosecond timescale. The equilibrium dispersion of the Yb *4f* and Rh *4d* states is explained by a *f-d* hybridization picture based on the periodic Anderson model. The transient dispersion is renormalized as function of optical excitation density. The hybridization gap displays a discontinuous change at an electronic temperature between 80 and 100 K. This temperature scale coincides with the onset of incoherent screening of the conduction band electrons and inelastic scattering with excited crystal electrical field levels.

Ultrafast spin density wave transition in Chromium governed by thermalised electron gas
Mon_ARPES1_4
Presented by Christopher Nicholson
Time- and angle-resolved photoemission spectroscopy is utilised to address the ultrafast dynamics of the antiferromagnetic spin density wave (SDW) transition photoexcited in epitaxial thin films of chromium. The complete destruction of SDW order on a sub-100 fs time scale is observed. We quantitatively extract the evolution of the SDW order parameter through the ultrafast phase transition and show that it is defined by the transient temperature of the thermalised electron gas. Our results reveal that equilibrium concepts such as the order parameter may be utilized even in the strongly non-adiabatic regime of ultrafast photo-excitation.

Session: Microscopy 1 (11:00-12:30, Auditorium E5)

Nanoscale tomography using coherent X-ray lensless imaging
Mon_Micro1_1
Presented by Manuel Guizar-Sicairos
Biological and artificial materials hinge on hierarchical structures for improved mechanical performance, and their characterization requires studies over length scales that span many orders of magnitude. While X-ray microscopy is well suited for studying moderately large volumes, it is challenging to manufacture efficient and well-corrected optics for nanoscale imaging. Ptychography is a form of X-ray coherent imaging that does away with imaging optics and provides nanoscale resolution. We will introduce the extension to 3D of this technique, describe recent advances in computational methods that allow improved resolution and faster acquisition speed, and outline current applications of the method.

Electron holography at high kinetic energies: from a case study to chemical selective imaging
Mon_Micro1_2
Presented Carsten Westphal
For more than half a century electron diffraction patterns have been considered as holograms of the local emitter environment. In the reconstruction, the step from the electron diffraction pattern to atom images turned out being rather difficult. In the optical case, holographic reconstructions had been very successful in the past. We present the main additional measures necessary for reconstructing electron holograms, in order to develop the method. In a next step, a more complicated system was reconstructed. Finally, we show that different elements can be identified within the emitter environment. All reconstructed images were obtained without any a-priori information.

The 3D shapes of spinning helium nanodroplets
Mon_Micro1_3
Presented by Bruno Langbehn
With the availability of femtosecond short-wavelength pulses at free-electron lasers (FEL), an insight into the structure of unsupported nanoparticles such as viruses or clusters has become feasible. While experiments using hard x-ray radiation push towards atomic resolution with small-angle scattering, in the soft x-ray and XUV regime full 3D information on the particle shape can be obtained from scattering images recorded up to large scattering angles. We have used intense XUV

pulses from the FERMI-FEL to image single helium nanodroplets. For non-spherical droplets the wide-angle scattering images clearly indicate prolate shapes, conflicting with previous results from the hard x-ray regime.

X-ray Fluorescence and Tomography Investigate Ancient Handwritten Manuscripts
Mon_Mircro1_4
Presented by Fauzia Albertin
X-ray tomography is finding a new and interesting application: the detection of text from inside unopened ancient documents. Potential advantages include the total absence of specimen damage and a large decrease of the digitization time. We present recent results including cases of text recognition from small documents (simulating folded Venetian testaments) and page-by-page ?virtual reading? of books with several hundred pages. In parallel, the research produced chemical results on inks used for administrative documents over six centuries - in particular, about the ubiquitous presence of iron and other heavy elements.

Session: XAS 1 – general (14:00-15:10, Auditorium E3)

X-ray based in-situ and ex-situ studies of chemical degradation phenomena in cultural heritage artefacts
Mon_XAS1_1
Presented by Koen Janssens
Many precious cultural heritage artefacts, consisting of a variety of heterogeneous materials (e.g., inorganic metal-sulfide pigments mixed with oil binders, applied in one or more layers) suffer from spontaneous degradation phenomena. For the detailed investigation of paintings, in recent years, we have found it useful to employ, next to analytical techniques suitable for microscopic 2D and 3D investigation of small fragments of these artefacts, also methods that provide chemical information on a larger scale. The use of macroscopic X-ray fluorescence (MA-XRF) and powder diffraction (MA-XRPD) imaging for examination of art works by Rubens, Van Gogh and Magritte will be discussed.

X-ray absorption spectroscopy in electrical fields: An element-selective probe of atomic polarization
Mon_XAS1_2
Presented by Verena Ney
We have studied a range of polar and nonpolar materials using x-ray absorption near-edge spectroscopy (XANES) in external electric fields. For polar materials an energy shift of the XANES by a few meV/kV is found which scales linearly with the applied voltage, while it is absent in non-polar or conducting materials. The energy shift of the XANES is different between two atomic species in one specimen and scales linearly with the atomic number of the studied element. Therefore, XANES in electrical fields opens the perspective to study atomic polarization with element specificity in a range of functional materials.

Probe-before-destroy Mn L-edge Absorption Spectroscopy of Photosystem II and Prototypical Mn Compounds
Mon_XAS1_3
Presented by Markus Kubin
The Photosystem II protein oxidizes water molecules in the Mn_4CaO_5 cluster after absorption of four visible photons. Details of the electronic and structural changes of the cluster necessary for this redox reaction are hitherto unresolved. We employ x-ray absorption spectroscopy at the Mn L-edge to probe the valence molecular orbitals of the Mn_4CaO_5 cluster. Femtosecond x-ray pulses probe the sample before x-rays damage it. Complementary spectra from structural mimics and simple Mn complexes in combination with multiplet and ab-initio calculations link the observable to the electronic structure of the Mn cluster. Mechanisms of sample damage by probing x-rays are addressed.

Session: Coincidence 1 (14:00-15:10, Auditorium E5)

Multielectron coincidence spectroscopy
Mon_Coin1_1
Presented by Pascal Lablanquie
We have developed a multielectron coincidence experiment in order to study multiple photoionization of atoms and molecules. Its power will be illustrated by a few selected examples including inner-valence Auger decays in K atoms, retrieval of Auger spectra resulting from core ionization of ions and study of double core hole formation and decay.

Experimental identification for an efficient neutralization pathway of the dication in a cluster
Mon_Coin1_2
Presented by Daehyun You
We report experimental identification for an efficient neutralization pathway of the dication embed in a cluster, using Ne-Kr mixed clusters as an example. When Ne^{2+} surrounded by Kr atoms is produced by Ne KLL Auger decay, electron-transfer-mediated decay (ETMD) of Ne^{2+}-Kr-Kr to Ne^{+}-Kr^{+}-Kr^{+} takes place emitting an ETMD electron. The process is identified by means of multifold electron-ion coincidence spectroscopy.

Ultrafast molecular three-electron collective Auger decay
Mon_Coin1_3
Presented by Raimund Feifel
Three-electron Auger decay is an elusive process, in which two outer-shell electrons simultaneously refill an inner-shell double vacancy with emission of a single Auger electron. Such transitions are forbidden in the lowest order by the many-electron selection rules, normally making their decay lifetimes orders of magnitude longer than those of normal Auger decay. Here we present compelling experimental and theoretical evidence for a much faster three-electron Auger decay of a molecular double inner-valence vacancy in CH_3F, and show that double inner-valence vacancies of molecular species can decay exclusively by this few-femtosecond ultrafast three-electron Auger process.

Session: XAS 2 – micro (15:45-16:55, Auditorium E3)

Characterization of Polymeric Materials with Soft X-rays
Mon_XAS2_1
Presented by Harald Ade
Spectroscopy is a key tool to probe the electronic structure of many systems, ranging from studies of fundamental interactions in correlated electronic and magnetic materials to bonding in organic compounds. When characterizing multi-phase multicomponent systems, the use of spectroscopy methods is often essential to provide contrast and discern structure and morphology with real space and reciprocal space methods. This combination of spectroscopy and spatial resolution has become a powerful tool that is making excellent contributions in many subdisciplines and towards solving important technological problems. We will trace some of the historical developments in soft x-ray spectro-microscopy and resonant scattering with a particular focus on the characterization of organic matter in general and organic semi-conducting devices in particular. Current efforts and future possibilities will be outlined.

Nanoscale phase separations in quantum materials
Mon_XAS2_2
Presented by Augusto Marcelli
The XANES spectroscopy is a unique powerful local and fast experimental method to study complex systems since it probes the nano-scale structure around selected atoms giving evidence for different local and instantaneous phases present in multi-scale highly correlated granular systems. Many recent experimental data have pointed out the presence of arrested phase separation and

the interplay of different phases occurring from nano- to micrometer-scale in transition metals and rare earth oxides systems. Actually, combining X-ray imaging at high spatial resolution with μ-XANES spectroscopy both mesoscale, nanoscale and atomic structural changes can be identified. This scenario opens the possibility to manipulate the mesoscopic phases to get new material functionalities.

Visualizing catalysis in X-PEEM with nanofabricated model surfaces
Mon_XAS2_3
Presented by Waiz Karim
Our work demonstrates top-down nanofabrication together with X-ray photoemission electron microscope (X-PEEM) to study catalytic metal nanoparticles and investigate the mechanism of hydrogen spillover, a critical phenomenon in heterogeneous catalysis. State-of-the-art nanolithography techniques are used to achieve well-defined metal nanoparticles down to six nanometers and in-situ visualization of chemical action is done at the single nanoparticle level. We give the first spectromicroscopic proof of hydrogen spillover using a novel model surface consisting of pairs of iron oxide and platinum particles positioned with unprecedented precision of one nanometer. These developments in nanocatalysis offer the possibility to unravel fundamental questions in catalysis.

Session: Coincidence 2 (15:45-16:55, Auditorium E5)

Revisiting the ultrafast dissociation of the O_2 molecule
Mon_Coin2_1
Presented by Xiao-Jing Liu
We explored the competition between the Auger electron emission and the molecular dissociation induced by the O1s→$3\sigma_\mu$* excitation in O_2. Several reaction mechanisms were identified: atomic Auger decay processes lead to O/O^+ fragments (ultrafast dissociation), while molecular Auger decays end up with either the O/O^+ pair or O^+/O^+ fragments. An interference pattern was observed in the electron-ion momentum correlation maps for the molecular decay, but not in the atomic case. Our experiment thus shows that the momentum transfer between a particle and a recoiling slit marks the path and destroys the interference.

Pairing correlated electrons from valence bands of solids: Double photoemission using MHz high-order harmonics
Mon_Coin2_2
Presented by Cheng-Tien Chiang
Interaction between electrons is the key ingredient of solid state physics ranging from magnetism, superconductivity to metal-insulator phase transitions as well as Kondo effect. Insights into the correlated electronic system can be obtained by double photoemission (DPE) spectroscopy, where two interacting electrons are emitted upon the absorption of one single photon. In this contribution we demonstrate DPE on the paradigmatic systems of the noble metal Ag(001) and the strongly correlated material NiO using a novel megahertz high-order harmonic light source. We attribute photoelectron pairs specifically to emission from sp as well as d bands and reveal their characteristic energy distribution.

Enhanced chiral asymmetries in the inner-shell photoionization of uniaxially oriented methyloxirane enantiomers
Mon_Coin2_3
Presented by Maurice Tia
We present here the first Photoelectron Circular Dichroism (PECD) measurements obtained on a partially oriented chiral molecule and supporting theoretical calculations. Our findings directly unravel that the delicate interplay of angular momentum of the circularly polarized photons and the diffraction of the emitted photoelectron wave by the molecular potential is at the heart of the phenomenon. Accordingly, the PECD effect is strongly enhanced as not randomly oriented

molecules but molecules which are partially oriented in space are investigated. These results make a major step towards a PECD measurement of “fixed-in-space” molecules where the asymmetry could in principle reach 100% and our work therefore paves the way for a detailed understanding of this fundamental photophysical process.

Tuesday, 5 July 2016

Plenary Source (9:00-10:15, Audimax F30)

The Extreme Light Infrastructure (ELI) project
Tue_Plenary_1
Presented by Dimitris Charalambidis
The Extreme Light Infrastructure (ELI) is a large scale research installation of the Roadmap of the European Strategy Forum for Research Infrastructures (ESFRI), published in 2006. Implemented as a distributed infrastructure, it aims to host some of the most intense lasers world-wide and secondary radiation and particle sources derived from them, develop new interdisciplinary research opportunities and make them available to an international scientific user community. In this presentation I will introduce the ELI project, will review on its implementation status, addressing the specific intricacies of each pillar and highlight selected examples of science that users can conduct in ELI.

Frontier research at FERMI
Tue_Plenary_2
Presented by Claudio Masciovecchio
The most recent light sources, extreme ultraviolet (EUV) and X-ray free electron lasers (FELs), have extended tabletop laser experiments to shorter wavelengths, adding element and chemical state specificity by exciting and probing electronic transitions from core levels. Through their unique properties, combining femtosecond X-ray pulses with coherence and enormous peak brightness, the FELs have enabled studies of a broad class of dynamic phenomena in matter that crosses many scientific disciplines and have led to major breakthroughs in the last few years.

Session: Microscopy 2 (11:00-12:30, Auditorium E3)

In situ soft X-ray microspectroelectrochemical studies of zinc-air battery materials
Tue_Micro2_1
Presented by Benedetto Bozzini
This talk aims at illustrating the contribution of in situ soft X-ray methods for shedding light on the properties of Zn-air batteries, concentrating on XRF, XAS and XPS microspectroscopy studies of air cathode catalysts and the anode performance of a model secondary battery, followed in situ by space- and time-resolved XRF and XAS.

Integration of structured illumination fluorescence microscopy with soft x-ray tomography at NSRRC
Tue_Micro2_2
Presented by Su-Yu Chiang
Structured illumination fluorescence microscopy (SIFM) is a super-resolution technique that enables improving the spatial resolution of a fluorescent image beyond the diffraction limit. Here, we will present the development of an SIFM system and its integration with a full-field transmission soft x-ray tomography (SXT) end station to provide complementary information for biomedical research at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan.

Spectroscopy and magnetism of magnetotactic bacteria studied by scanning soft X-ray microscopy and ptychography
Tue_Micro2_3
Presented by Adam Hitchcock
Scanning Transmission X-ray microscopy (STXM) and ptychography have been used to investigate spectroscopy and magnetism at the individual magnetosome level of Magnetovibrio blakemorei strain MV-1 magnetotactic bacteria. The improved spatial resolution and spectral intensity of

ptychography over conventional STXM is documented. Observations of a dividing cell as well as statistical studies of magnetic moment orientation relative to the single flagellum of MV1 cells are used to gain insights into how these species pass on the correct magnetic orientation in the process of cell division.

Hard X-ray Magnetic Imaging at the Nanoscale with Dichroic Ptychography
Tue_Micro2_4
Presented by Claire Donnelly
Nanoscale investigations of magnetic configurations are key to understanding the influence of the material microstructure on the magnetic properties of a material. Until now, X-ray magnetic microscopy at the nanoscale has been limited to the investigation of surfaces and thin films. Here we present hard X-ray magnetic imaging at the nanoscale, achieving a 50x increase in the achieved spatial resolution. We perform dichroic ptychography, a coherent diffractive imaging technique, and image the magnetic configuration of a micrometre-thick FeGd multilayer. This advance in hard X-ray magnetic imaging will enable the detailed investigation of buried magnetic structures and extended 3D magnetic systems.

Session: PES 1 – AMO (11:00-12:30, Auditorium E5)

Electron spectroscopy of isolated atoms and molecules by using hard X-ray photons
Tue_PES1_1
Presented by Ralph Püttner
Recently a Hard X-ray Photoelectron Spectroscopy (HAXPES) set-up for gas-phase measurements with unique conditions in terms of experimental resolution and photon flux became operational at the GALAXIES-beamline of the synchrotron radiation facility SOLEIL in France. Using this set-up, we present measurements of the Ar $1s^{-1}2p^{-1}nl$ double core hole (DCH) shake-up states observed with conventional single-channel photoelectron spectroscopy as well as a study of DCH states in the molecules SiX_4 with X = F, Cl, Br, and CH_3. Finally, electronic state lifetime interference contributions in the resonant KLL Auger spectra of HCl and CH_3Cl are discussed.

Spectroscopy and dynamics of double-core-hole states in neon
Tue_PES1_2
Presented by Marc Simon
Using synchrotron radiation and high-resolution electron spectroscopy, we identified double K-shell hole states in neon, and namely $1s^{-2}V$ states, corresponding to simultaneous 1s ionization/1s→V excitation. The lifetime broadening of the Double Core Hole (DCH) states and the relative cross sections of direct and conjugate shakeups have been measured and compared to ab initio calculations. The hypersatellite Auger spectrum has been measured and assigned in detail. Post Collision Interaction due to unequal energy sharing of the two core electrons is observed in the hypersatellite spectrum. The angular distribution of the photoelectrons emitted in the creation of $1s^{-2}V$ states has been determined.

Reconstruction of molecular wave functions from angular-resolved photoemission data
Tue_PES1_3
Presented by Pavel Kliuiev
We discuss the means of how both the magnitude and the phase of a molecular electronic wave function can be reconstructed from angular-resolved photoelectron spectroscopy (ARPES) data. We draw an analogy between the phase problem in molecular orbital imaging via ARPES and of that in optical coherent diffraction imaging, and we present the reconstructed molecular wave functions from simulated and experimental ARPES data as well as the micrometer-sized structures from an analogue optical experiment.

Dynamical effects in the valence photoionization of CO_2
Tue_PES1_4

Short abstracts of talks

Presented by Saikat Nandi
When passing through two spatially separated slits with a separation comparable to the wavelength, optical waves can interfere to produce characteristic fringes. Similarly, quantum particles, coherently emitted from two sources, can interfere with each other owing to their wave nature. The current study is the very first attempt to explore quantum interference with electrons in case of a triple slit: the CO_2 molecule. The signature of this effect seems to appear in the branching ratios for different vibrational sub-states for selected electronic states in CO_2 which show clear deviation from the predicted Franck-Condon values as a function of incident photon energy.

Session: RIXS 1 - TMO (14:00-15:10, Auditorium E3)

Revealing the electronic ground state of $ReNiO_3$ combining high-resolution Ni-L_3 X-ray absorption and resonant inelastic X-ray scattering
Tue_RIXS1_1
Presented by Valentina Bisogni
A comprehensive spectroscopic study of $ReNiO_3$ is presented, by taking $NdNiO_3$ as a representative example. We combined for the first time X-ray Absorption (XAS) and high-resolution Resonant Inelastic X-ray Scattering (RIXS) at the Ni L_3 edge and we reveal an unusual coexistence of bound and continuum excitations in the GS of these materials, providing a strong evidence for the abundance of O 2p holes. Using cluster calculations and Anderson impurity model interpretation, we show that the orbital excitations and the energy dispersing spectral signatures arise consistently from a Ni 3d8 configuration along with holes in the O 2p valence band.

Resonant x-ray emission spectroscopy study of epitaxial strain effects on spin states of Co ions in $LaCoO_3$ thin films
Tue_RIXS1_2
Presented by Yuichi Yokoyama
We investigated the spin states of $LaCoO_3$ thin films grown on LSAT: $(LaAlO_3)_{0.3}(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ substrates by resonant x-ray emission spectroscopy and hard x-ray photoelectron spectroscopy at SPring-8. By comparing the obtained results with those of bulk single crystals, the spin state is considered to change from low-spin to intermediate-spin and/or high-spin states by epitaxial strain effects from LSAT substrates. In addition, the high-spin population increases as the temperature increases. Our study shows firstly by direct observation of the electronic structures that the epitaxial strain can control the spin states of $LaCoO_3$.

Weak Ferromagnetism in α-Fe_2O_3 Studied by Magnetic Circular Dichroism in SX-RIXS
Tue_RIXS1_3
Presented by Jun Miyawaki
α-Fe_2O_3 exhibits weak ferromagnetism due to Dzyaloshinskii-Moriya interaction at temperatures between the Morin transition and Néel temperature. We measured and calculated MCD in SX-RIXS to investigate the origin of the weak ferromagnetism. Although MCD in XAS was not detected, MCD in RIXS was clearly observed for the *dd* transition at 1.8 eV loss energy depending on the excitation energy and crystal orientation. The results indicate that the observed MCD in RIXS was originated from the RIXS process and the intermediate states in RIXS excited to the charge transfer transition play a key role in the magnetic order.

Session: Sources 1 (14:00-15:10, Auditorium E5)

MAX IV as example of the potential of diffraction limited storage rings
Tue_Sources1_1
Presented by Jesper Andersen
Recent breakthroughs have facilitated the design of storage rings with very low emittance and consequently high brightness opening the possibility of reaching the ultimate diffraction limit even at hard X-ray energies. Such diffraction limited storage rings open up a number of new

opportunities for X-ray methods. In this talk I will use the MAX IV Laboratory as example of what can be achieved with these new sources. An overview will be given of the beamlines under construction and envisioned at the facility and the science these will facilitate with special emphasis on the low emittance of the MAX IV facility. Finally, a brief overview of the operational status of the facility will be given.

Inner-shell multi-color x-ray lasing and two-photon absorption driven by ultra-intense femtosecond XFEL pulses
Tue_Sources1_2
Presented by Joanna Hoszowska
Interaction of ultra-intense femtosecond hard x-ray free-electron laser (XFEL) pulses with solid Fe was explored by means of the high-resolution x-ray emission spectroscopy technique. The experiment was performed at the CXI end-station of the Linac Coherent Light Source (LCLS). The focused x-ray beam provided extreme peak power densities reaching ~10^{20} W/cm^2. Multi-color hard x-ray lasing based on the inner-shell transition scheme was established, and the nonlinear two-photon absorption leading to K-shell hollow atom formation and to single K-shell ionization of solid Fe was observed.

Mg $L_{2,3}$ stimulated emission from MgO pumped by FERMI FEL pulses: a milestone toward a soft-x-ray solid-state laser
Tue_Sources1_3
Presented by Philippe Jonnard
We show evidence, both experimentally and theoretically, for stimulated emission of Mg $L_{2,3}$ from a MgO solid target pumped by extreme ultraviolet pulses delivered by the FERMI free electron laser (FEL) facility in Trieste (Italy). We observed in backward geometry two effects separately revealed in semiconductors and metals: the stimulated emission process is enhanced in a privileged direction and its intensity exhibits a material- dependent threshold characteristic of the spontaneous amplified emission regime. Our results could represent a milestone for future soft-x-ray solid-state lasers.

Session: RIXS 2 Corr Mat (15:45- 16:55, Auditorium E3)

High-Resolution Soft X-ray Inelastic Scattering and Coherent Diffraction Imaging
Tue_RIXS2_1
Presented by Di-Jing Huang
We will present an overview of soft X-ray scattering at the Taiwan Photon Source. To improve the efficiency of RIXS measurements, the energy compensation principle has been adopted for the dispersions of monochromator and spectrometer. After constructing the proof-of-principle RIXS setup, we designed a new RIXS beamline using a novel 25-ridge grating bender system. For the coherent scattering branch, a soft X-ray spectro-microscope system using Kirkpatrick-Baez (KB) will be presented. We will discuss the design and the expectation of this new beamline, test results for studying strongly correlated electron materials with spectroscopic information at the nanoscale.

Direct observation of crystal field splitting of 4f levels by Resonant Inelastic soft X-ray Scattering
Tue_RIXS2_2
Presented by Andrea Amorese
The last years' improvement in the energy resolution of Resonant Inelastic soft X-ray scattering (soft-RIXS) opened up the possibility of studying new excitations. Among these, electronic excitations within the 4f shell can now bring much information about the properties of lanthanides' compounds. In Cerium intermetallic compounds of the "122" family, 4f levels can hybridize with surrounding atoms' wavefunctions leading to peculiar physical properties, whose full understanding requires the knowledge of the 4f levels' splitting and symmetry. We will present high resolution measurements on these compounds, demonstrating for the first time the ability of soft-RIXS to probe 4f levels' scheme.

Short abstracts of talks

Probing the electron-phonon coupling in high-temperature superconductors using ultrahigh resolution Resonant Inelastic X-ray Scattering
Tue_RIXS2_3
Presented by Laura Chaix
Uncovering the mechanism of high temperature superconductivity in cuprates remains an important question in condensed matter physics.
While spin fluctuations may be crucial for forming superconductivity in cuprates, abundant experimental observations also demonstrate a strong electronic coupling to the lattice. It is still debating whether the phonons also play a role in the pairing mechanism. Resonant inelastic X-ray scattering (RIXS) measurements on cuprate compounds provide opportunities to probe both magnetic and charge excitations in the energy and momentum space, which may shed new light on the cuprate problems.

Session: Sources 2 (15:45, 16:55, Auditorium E5)

High-accuracy deep-ultraviolet Ramsey-comb spectroscopy of krypton and molecular hydrogen
Tue_Sources2_1
Presented by Kjeld Eikema
Precision spectroscopy at deep ultraviolet and shorter wavelengths is typically hampered by a lack of suitable laser sources. We show that this issue can be solved by using the Ramsey-comb method, based on excitation with pairs of amplified and phase-controlled ultrafast laser pulses from a frequency comb laser. The pulse energy (mJ-level) enables easy upconversion to the deep ultraviolet, resulting in two-photon excitation of krypton with 108 kHz accuracy at 212 nm, and the first Ramsey-comb excitation of molecular hydrogen on the EF-X transition at 202 nm.

Single shot NEXAFS investigations of biological samples in the soft X-ray region using a Laser Produced Plasma Source
Tue_Sources2_2
Presented by Katharina Witte
X-ray absorption spectroscopy (XAS) with soft X-ray radiation gives the possibility to investigate K edges of light element and is a common method to analyze structural and chemical properties e.g. of biological samples. We present a laser produced plasma source for the soft X-ray region between 80-1200 eV with an optimized spectrometer for high resolution near edge X-ray absorption fine structure (NEXAFS) investigations. With this setup single shot NEXAFS measurements within 1 ns are feasible. NEXAFS spectra of Cu-Chlorophyllin molecules are shown and compared to theoretical DFT calculations to assign characteristic features to chemical constituents of the sample.

High precision laser spectroscopy of highly charged ions: Resonant excitation of Li-like Kr^{33+} at 136 eV and perspectives for hyperfine structure studies at highest Z with FLASH
Tue_Sources2_3
Presented by Günter Brenner
We report on high-resolution spectroscopy measurements of the $2\ ^2S_{1/2} - 2\ ^2P_{3/2}$ fine-structure transition of Li-like Kr^{33+} ions trapped in an electron beam ion trap (EBIT) and resonantly excited by soft X-ray photons at 136 eV produced by the Free Electron Laser in Hamburg FLASH. The result of 136.189(6) eV with an accuracy of below 50 ppm improves the so far best measurement value by a factor of 6 in excellent agreement with recent QED calculations. We will also discuss the perspectives for hyperfine structure studies in heavy Li-like systems like Bi^{80+}.

Wednesday, 6 July 2016

Plenary Theory (9:00-9:45, Audimax F30)

On the developments for a complete theory of RIXS in strongly correlated systems
Wed_Plenary_1
Presented by Thomas Devereaux
In this talk I will present a review of the current status of the theory of resonant inelastic x-ray scattering, with a particular focus on what can be learned about fundamental multi particle excitations in strongly correlated materials. I will emphasize these developments in concert with the improved ability of new light sources to offer exquisite mapping of excitations in the frequency and time domain with full polarization control.

Recoil and Rotational Doppler effects in Molecular Photoionization
Wed_Plenary_2
Presented by Faris Gel'mukhanov
The ability to rotate molecules offers ways to control nuclear motion with important applications in science. Commonly, high power lasers are employed to induce super-rotation using the optical centrifuge technique. We suggest an alternative scheme to spin-up molecules to fast rotation in which high angular momentum can be transferred almost instantaneously in the course of hard X-ray ionization accompanied by a recoil effect.

Session: ARPES 2 - surf. (11:00-12:20, Auditorium E3)

Study of structural dynamics by means of time- and angle-resolved photoelectron spectroscopy and diffraction
Wed_ARPES2_1
Presented by Matthias Hengsberger
Photoelectron angular intensity distributions contain information about the electronic and atomic structure in surfaces. The method relies on interference of directly emitted and scattered electron waves, which produces a complex pattern from which the atomic environment of the emitter can be deduced. When used with pulsed light in a pump-probe setup structural dynamics can be studied in detail. Results of coherent phonon excitations in Bi will be presented. We demonstrate how electronic and structural degrees of freedom can be disentangled allowing the relative timing of phonons and electronic structure modulations to be determined with great precision.

C_{1h} symmetry induced non-vortical Rashba spin structure
Wed_ARPES2_2
Presented by Kazuyuki Sakamoto
In this paper, we report a totally novel spin structure found on a Tl/Si(110)-(1x1) surface with C_{1h} symmetry by spin- and angle-resolved photoelectron spectroscopy. The constant energy contour of the upper Rashba-Bychkov split band has a warped elliptical shape centered at a point without time-reversal symmetry, and the spin-polarization vector of this state is in-plane and points the same direction along the whole elliptic contour. This novel RB spin structure is confirmed as a general phenomenon originating from the C_{1h} symmetry by first-principles theoretical calculations, and can be explained by a simple picture based on the symmetry of the surface.

Two-dimensional hole gas at ferroelectric $BaTiO_3$ film surfaces
Wed_ARPES2_3
Presented by Stefan Muff
In our experiments, we studied films of $BaTiO_3$ grown on different substrates. PFM measurements prove the ferroelectricity of our samples with a preferred polarization along the out of plane direction. By using ARPES we directly map the existence of metallic states at the clean surface of our films. The conducting states consist of heavy electron-like bands with a three-dimensional

dispersion as well as surface confined 2D states. These 2D states show, in contrast to the 2D electron like states observed at the surface of the closely related compounds $SrTiO_3$ and $KTaO_3$, a hole like dispersion.

Observation of the dynamics of charge separation at donor/acceptor interfaces in organic photovoltaics
Wed_ARPES2_4
Presented by Friedrich Roth
Photo-induced generation, migration, exchange, and trapping of charge carriers at interfaces between solids, molecules, and liquids, and in nanoscale heterojunction structures are of central importance for the vast majority of emerging solar energyconversion technologies. Here, we report the site-specific probing of the charge transfer dynamics in a prototype system for organic photovoltaics (OPVs), consisting of Copper-Phthalocyanine (CuPc) and C_{60}, by picosecond time-resolved X-ray photoelectron spectroscopy (tr-XPS). Charge transfer from the electron donor (CuPc) to the acceptor (C_{60}) and subsequent charge carrier daynamics are monitored by recording the time dependent C 1*s* core level photoemission spectrum of the system.

Session: RIXS 3 (11:00-12:30, Auditorium E5)

New perspectives in inelastic x-ray scattering – UPBL6@ID20
Wed_RIXS3_1
Presented by Marco Moretti
In the frame of the ESRF Upgrade – Phase I, the UPBL6 project aimed at the construction of a state-of-the-art hard inelastic x-ray scattering (IXS) beam line on undulator port ID20. The beam line is now operational and fully dedicated to the study of electronic and magnetic excitations in condensed matter. Scientific goals comprise the investigation of strongly correlated electron systems, functional materials, and chemical reactions in liquids and gases.

Disentangling orbital and magnetic contributions to the exotic Spin Peierls transition in $TiPO_4$
Wed_RIXS3_2
Presented by Marcus Dantz
Understanding the correlation between spin, orbital and lattice degrees of freedom is one of the most challenging tasks in modern solid state physics. Quasi one-dimensional magnetic systems are of special interest in this aspect because of intriguing properties that emerge from the reduced dimensionality such as fractionalization of an electron's degrees of freedom into several independent quasiparticles, large electron phonon coupling due to low electronic screening and instability towards Peierls-like dimerization. Here, we investigate $TiPO_4$ using resonant inelastic x-ray scattering in order to unravel the interplay of those degrees of freedom involved in its exotic spin-Peierls transistion.

Imaging Anti-Ferromagnetic A-type domains in strongly correlated $LaSr_2Mn_2O_7$
Wed_RIXS3_3
Presented by Mirian Garcia-Fernandez
We report a soft x-ray nanodiffraction study of antiferromagnetic domains in the strongly correlated bilayer manganite $La_{0.96}Sr_{2.04}Mn_2O_7$.We find that the antiferromagnetic domains form a unique domain pattern with each domain having an intrinsic memory of its spin direction. This can be explained by the presence of crystallographic or magnetic imperfections locked in during the crystal growth process which pin the antiferromagnetic domains. The antiferromagnetic domain pattern shows two distinct types of domains. One of the domain types was observed to contain a periodic ripple in the manganese spin direction with a period of approximately 4 μm.

Quantification of 'Invisible' CoO by *in-situ* 2p3d Resonant Inelastic X-ray Scattering
Wed_RIXS3_4
Presented by Boyang Liu

Short abstracts of talks

2p3d RIXS offers superior power to reveal the minority species 'invisible' in 2p XAS. In this work, carbon nanotubes supported cobalt Fischer-Tropsch (FT) catalysts are chosen as a model system to study its activation process. Twelve 2p3d RIXS datasets obtained consistently at four excitation energies at three temperatures are decomposed into CoO and Co features by holistic fitting, and the spectral intensity ratio is converted into the species ratio. RIXS quantification results demonstrates that, despite an almost pure cobalt metal signal from XAS, still less than 10% of the cobalt is present as CoO at the highest activation temperature.

Session: XAS 3 – timeresolved (14:00-15:40, Auditorium E3)

Time-resolved x-ray detected-ferromagnetic resonance
Wed_XAS3_1
Presented by Gerrit van der Laan
Recently, x-ray detected FMR (XFMR) has emerged as a powerful synchrotron radiation based tool able to study the element-selective magnetization dynamics. Magnetic and chemical contrast in XFMR is obtained by x-ray magnetic circular dichroism (XMCD), while the phase difference of the magnetization precessions is monitored using a stroboscopic measurement technique. A unique property of time-resolved XFMR is the visualisation of the magnetization precession of each individual layer in a magnetic device. The measured amplitude and phase response of the magnetic layers allow for a clear signature of spin transfer torque (STT) coupling due to spin pumping.

Multi-element probing of ultrafast demagnetization dynamics with high harmonics of an intense femtosecond IR laser
Wed_XAS3_2
Presented by Boris Vodungbo
High harmonic generation sources are powerful tools for the investigation of ultrafast dynamics. In addition to providing ultra-short, inherently jitter-free pump and probe pulses, the emitted harmonics span a large spectrum which covers a broad range of absorption resonances of different elements. This enables simultaneous probing of the individual dynamics of different components of complex materials. We apply this technique to investigate the role of superdiffusive spin transport in ultrafast demagnetization dynamics of transition metal multilayer and ferrimagnetic transition metal rare earth alloys.

Element-selective investigation of the spin dynamics in Ni_xPd_{1-x} magnetic alloys in the extreme ultraviolet spectral range
Wed_XAS3_3
Presented by Roman Adam
We present element-selective studies, using extreme ultraviolet (XUV) light, to gain insight into the spin dynamics in Ni_xPd_{1-x} magnetic alloys on the femtosecond time scale. In order to tune the exchange interaction strength as well as the spin-orbit coupling we varied the composition of Ni_xPd_{1-x} alloys in 100<x<50 range. Transversal MOKE (T-MOKE) employing laser-driven high harmonic source generating light in the extreme ultraviolet range (40-72eV) was then employed to measure the ultrafast demagnetization at both Ni $M_{2,3}$- and Pd N_3-edges element-selectively. Our results provide deeper insight into the strength of the exchange coupling between Pd and Ni in Ni_xPd_{1-x} alloys.

Nonthermal symmetry-broken states and nonequilibrium criticality in correlated lattice models
Wed_XAS3_4
Presented by Philipp Werner
We study the dynamics of correlated lattice systems, which are driven out of a symmetry-broken phase, using the nonequilibrium generalization of dynamical mean field theory. Trapping in nonthermal ordered states is observed in strongly correlated antiferromagnetic insulators and linked to the long thermalization time of doublons and holes. In the weak-coupling regime, we find clear evidence for a relaxation controlled by a nonthermal fixed point. The universality of the latter

concept is illustrated with results for phonon-mediated superconductors and excitonic insulators.

Session: ARPES 3 (14:00-15:40, Auditorium E5)

Layer-dependent quantum cooperation of electron and hole states in the anomalous semimetal WTe_2
Wed_ARPES3_1
Presented by Ivana Vobornik
We report angle and spin-resolved photoemission spectroscopy of WTe_2 transition metal dichalcogenide with titanic nonsaturating magnetoresistance. Supported by first-principles calculations and high-resolution surface topography, we reveal the existence of a layer-dependent electronic behaviour. The balance of electron and hole states which is believed to lead to nonsaturating magnetoresistive behaviour, is found only when considering at least three Te-W-Te layers, showing that the behavior of WTe_2 is in between those expected for 2D and 3D electronic systems.

Quasi 2D electronic states with high spin-polarization in centrosymmetric MoS_2 bulk crystals
Wed_ARPES3_2
Presented by Mathias Gehlmann
Time reversal symmetry dictates that nonmagnetic, centrosymmetric crystals cannot be spin-polarized as a whole. However, it has been recently shown that the electronic structure in these crystals can in fact show regions of high spin-polarization, as long as it is probed locally in real and in reciprocal space. Using spin-ARPES and DFT calculations we demonstrate that distinct valleys in the electronic band structure of MoS_2 bulk crystals are highly spin-polarized and almost completely confined within two dimensions. Our findings prove that these highly desired properties of MoS_2 can be accessed without thinning it down to the monolayer limit.

Revealing the bond disproportionated insulating phase in the high-T_c superconductor parent compound $BaBiO_3$
Wed_ARPES3_3
Presented by Nicholas Plumb
We reveal the band structure of $BaBiO_3$, an insulating parent compound of doped high-T_c superconductors, using *in situ* angle-resolved photoemission spectroscopy (ARPES) on thin films grown by pulsed laser deposition (PLD). The experiments essentially confirm a “bond disproportionation” picture of the insulating phase, which carries important implications for understanding the doping dependence and superconductivity in bismuthates, and may have connections to other systems, such as the rare earth nickelates.

Realization of a vertical topological p-n junction in epitaxial Sb_2Te_3/Bi_2Te_3 heterostructures
Wed_ARPES3_4
Presented by Lukasz Plucinski
We present a direct experimental proof by angle-resolved photoemission of the realization of a vertical topological p-n junction made of a heterostructure of two different binary 3D TI materials Bi_2Te_3 and Sb_2Te_3 epitaxially grown on Si(111). We demonstrate that the chemical potential is tunable by about 200meV when decreasing the upper Sb_2Te_3 layer thickness from 25 to 6 quintuple layers without applying any external bias. These results make it realistic to observe the topological exciton condensate and pave the way for exploring other exotic quantum phenomena in the near future.

X-ray spectroscopy applied to structure and dynamics of interfaces in transition-oxide-based stacks studies
Wed_ARPES3_5
Presented by Elena Filatova
Comprehensive approach to study of transition-metal-oxide-based systems focusing on the study of

both the structure of active layers and processes occurring at the interfaces between oxide and active metal is presented. Of particular interest is a study of oxygen scavenging process from the oxide and conditions provoking this process. Particularly, the oxygen scavenging by chemically active metals from γ-Al_2O_3 generates a high density of gap states in the insulating oxide near the metal surface and the formation of polarization layer in the electrode. Also the effect of thin interlayer insertion on the structure and extension of the interface is discussed.

Thursday, 7 July 2016

Plenary Time Resolved Spec. (9:00-9:45, Audimax F30)

Atomic, molecular, and nuclear quantum dynamics in (strong) visible, VUV and x-ray fields
Thu_Plenary_1
Presented by Thomas Pfeifer
What happens to the constituents of matter and their properties when you expose them to intense light fields? Can absorption be transformed into emission within a few femtoseconds, in the absence of inversion? Will intense lasers allow a new kind of chemistry?

Session: PES 2 (11:00-12:30, Auditorium E3)

Photoelectron Circular Dichroism (PECD) on chiral systems: a fine probe of photoionization dynamics and molecular structures
Thu_PES2_1
Presented by Laurent Nahon
Photoelectron circular dichroism (PECD) manifests itself as an intense forward/backward asymmetry in the angular distribution of photoelectrons produced from randomly-oriented enantiomers of a chiral system photoionized by circularly-polarized light. This chiroptical orbital-specific effect is a sensitive probe of both photoionization dynamics and of static molecular structures such as isomers, conformers, clustering as well as vibration dynamics. Recent PECD results, on showcase chiral systems as well as on the amino acid alanine, obtained with the high resolution variable polarization VUV beamline DESIRS at SOLEIL, will be presented.

Probing the VUV photoionisation of methyl radicals produced in a pyrolysis and a reactor sources
Thu_PES2_2
Presented by Christian Alcaraz
We report on the production of vibrationally and electronically excited methyl cations, CH_3^+, from the VUV photoionisation of methyl radicals, CH_3, on the DESIRS beamline at the French synchrotron SOLEIL, our main motivation being to study the effect of the excitation of CH_3^+ ions on their reactivity. The goal was also to compare two complementary sources of CH_3 radicals which were formed in a beam either by pyrolysis of precursor molecules (CH_3NO_2 or CH_3NNCH_3) passing through a heated SiC tube or reaction of F atoms with CH_4, in a fast flow tube reactor (SYNCROKIN project).

Catalysis, photovoltaics, & hydrogen-storage related nanoparticles as seen by photoelectron spectroscopy
Thu_PES2_3
Presented by Maxim Tchaplyguine
Unique information can be obtained when synchrotron-based photoelectron spectroscopy is applied to free multicomponent nanoparticles. In the work being reported three classes of nanoparticles have been studied, with their electronic structure and component distribution characterized at atomic monolayer resolution: 1) catalysis-relevant nanoparticles containing gold, silver, or copper oxides. 2) variable-gap semiconductor nanoparticles actual for the Quantum Dot Solar Cells, containing PbS. and 3)hydrogen-storage relevant nanoparticles, containing Mg-hydride.

Temperature dependence of the partially localized state in molecular network
Thu_PES2_4
Presented by Olha Popova
2D organic and metal-organic nanoporous networks can scatter surface electrons, leading to their partial localization inside the pores. Such quantum states are related to intrinsic surface states of the substrate material. Stable nanoporous coordination networks generated by a Perylene derivative (DPDI) on Cu(111), in particular, have been reported to trap surface electrons and to give

rise to a new band structure. In the present work we use angle-resolved photoemission (ARPES) that both, Shockley and partially localized states shift by the same amount to higher binding energy upon changing temperature of the sample. To address the origin of the confined state, we study its temperature dependence in comparison to the surface state of the pristine surface. We observe that both states simultaneously shift to higher binding energies when decreasing the sample temperature. This result evidences that the reported confined state originates from the Shockley state.

Session: Theory (11:00-12:30, Auditorium E5)

Resonant inelastic x-ray scattering: theory, experiments, and its impact on the understanding of correlated matter
Thu_Theo_1
Presented by Krzysztof Wohlfeld
Recently resonant inelastic x-ray scattering (RIXS) has positioned itself as one of the main spectroscopic techniques which is used to understand the complex states of matter. In this talk, after giving a basic theoretical understanding of RIXS, I will explain the reasons behind its recent successes. Thus, I will give a brief overview of some of the most spectacular RIXS experiments and describe their profound impact on the theoretical understanding of the correlated electron systems.

First-principles simulations of X-ray absorption spectroscopy at energy-relevant materials interfaces
Thu_Theo_2
Presented by David Prendergast
X-ray absorption spectroscopy is increasingly the tool of choice to provide element-specific local chemical information relevant to energetic processes at embedded material interfaces. However, the direct interpretation of these spectra requires an atomistic structural and dynamical model for clear insight into energy transfer mechanisms. We employ first-principles methods based on density functional theory to predict the importance of dynamics and environmental or interfacial effects on X-ray absorption spectra of condensed phase interfaces and have recently applied this approach to problems in the field of electrical energy storage.

Interaction between localized and itinerant states - excitons, resonances and band excitations in time and frequency domain
Thu_Theo_3
Presented by Maurits W. Haverkort
Depending on the amount of correlations, spectra manifest themselves as local excitons with multiplets, edge singularities, resonances, or the density of states. Both extremes, i.e. local excitons or non-interacting delocalized excitations are theoretically well under control. Describing the intermediate regime, where local many body interactions and band- formation are equally important is a challenge. For this purpose we developed a post density functional theory method merging ideas from density renormalization group and quantum chemistry. It allows us to calculate a variety of different spectroscopy types, both in the frequency as well as the time domain. Implementations are online available at http://www.quanty.org.

Efficient Bethe-Salpeter equation calculations of X-ray spectra
Thu_Theo_4
Presented by Keith Gilmore
The Bethe-Salpeter equation (BSE) is a highly accurate, many-body approach to calculating x-ray and optical spectra from first-principles. However, the method is computationally intensive and heretofore limited to systems of modest size. We have recently implemented an efficient solution of the BSE for x-ray absorption, x-ray emission, and both resonant and non-resonant inelastic x-ray scattering spectra on systems up to 500 atoms [Comp. Phys. Comm. 197, 109 (2015)]. We

demonstrate the capabilities of our code by reproducing with great fidelity the x-ray absorption spectrum of crystalline C60 measured with high energy resolution.

Session: ARPES 4 Met (14:00-15:20, Auditorium E3)

Highly-Efficient Parallel Spin Filtering in a Time-of-Flight Momentum Microscope
Thu_ARPES4_1
Presented by Gerd Schönhense
A time-of-flight (ToF) momentum microscope has been equipped with an imaging spin filter that enables a simultaneous measurement of more than 10,000 data points. This as-yet-unachievably rapid access to spin textures is exploited in a new set-up at BESSY II. Anomalous surface states on W(110) exhibit Dirac-like dispersion and spin texture. Electronic bands in ferroelectric GeTe(111) reveal Rashba splitting of surface and bulk bands with opposite spin helicity of the inner and outer Rashba bands. Spin-polarized one-step photoemission calculations show excellent agreement with the experiments.

k-resolved electronic structure by soft-X-ray ARPES: From 3D systems to buried interfaces and impurities
Thu_ARPES4_2
Presented by Vladimir N. Strocov
The spectroscopic power of soft-X-ray ARPES, employing photon energies around 1 keV, arises from enhancement of the photoelectron escape depth compared to the conventional VUV-ARPES, concomitant sharp definition of the 3D electron momentum, and resonant photoexcitation delivering elemental and chemical state specificity. Advanced instrumentation at the Swiss Light Source has allowed SX-ARPES to develop from the traditional applications to 3D bulk crystals to the most photon-hungry cases of buried interfaces and impurities, and even intervene there into the domain of quasiparticle interaction. We overview this development vector with the most recent highlights extending from bulk materials to buried systems.

An x-ray standing-wave study of the high-T_c superconductor $Bi_2Sr_2CaCu_2O_8$
Thu_ARPES4_3
Presented by Cheng-Tai Kuo
The cuprate high-T_c superconductors are still not fully understood. Here we present an x-ray standing-wave (SW) photoemission study of the classic cuprate, $Bi_2Sr_2CaCu_2O_8$ in its Bi2212 form, in order to provide a unique type of depth resolution for the several atomic planes in the lattice: Cu-O, Ca-O, Sr-O, and Bi-O. Core-level photoelectron rocking curves were acquired as a function of incidence angle around the (002) Bragg diffractions, and they show distinct shapes from the different atomic planes, which further agree well with atomic-level dynamical x-ray diffraction calculations. Future SW ARPES measurements will be discussed.

Dynamics of Space-Charge Acceleration- Auger- and Photo Electrons Emitted From a Cu(111) Surface
Thu_ARPES4_4
Presented by Gregor Schiwietz
The so-called vacuum space-charge acceleration of electrons is investigated experimentally and theoretically for ejected electrons due to X-rays of a few hundred eV during intense infra-red laser excitation. Electron spectra have been taken at the BESSY II slicing facility for grazing-incidence photons interacting with an atomically clean Cu(111) surface. The influence of high ionization densities on the properties of Auger and photo electrons liberated by a probe X-ray beam is investigated in time-resolved pump and probe measurements. Strong electron-energy shifts have been found and assigned to space-charge acceleration.

Session: Time res. 1 (14:00-15:30, Auditorium E5)

Short abstracts of talks

Coherent control experiments at the FERMI FEL
Thu_Time1_1
Presented by Denys Iablonskyi
We demonstrate and exploit the longitudinal coherence of two-colour extreme ultraviolet (XUV) light from the FERMI seeded Free Electron Laser (FEL). The phase difference between two wavelengths was controlled by an electron delay line, installed between undulators emitting different colours, with 3 attoseconds resolution. Interference as a function of relative phase was observed between two ionization pathways, one-photon ionization by the second harmonic and two-photon ionization by the first harmonic. We also propose another novel scheme of interference which utilizes the full coherence of FERMI FEL.

Attosecond time-resolved photoelectron spectroscopy of liquids
Thu_Time1_2
Presented by Inga Jordan
Attosecond spectroscopy has offered promising insights into ultrafast dynamics in solid and gas-phase systems, but has not been extended to the liquid phase yet. We report the achievement of this fundamental advance and demonstrate the measurement of attosecond photoionization delays from liquid water. In combination with theory, these delays reveal electron propagation effects through the aqueous environment and dephasing processes. These results are expected to provide new insights into the nature of photoionization and electron transport in liquid water.

Laser assisted photoelectric effect from liquids
Thu_Time1_3
Presented by Christopher Arrell
The laser assisted photoelectric effect (LAPE) has been observed and characterised from liquid water for the first time. Photoelectrons from the first three molecular orbitals of liquid water and from the vapour surrounding the sample, excited by a 36 eV pulse and subsequently dressed with an 800 nm laser pulse, were collected and their time dependent intensity redistribution recorded. A genetic algorithm was used to abstract the LAPE response with good agreement found with theory. Clear sidebands from both the liquid and gas phase were observed.

Ultrafast relaxation dynamics of ethylene ionized by XUV attosecond pulses
Thu_Time1_4
Presented by Matteo Lucchini
Ethylene (C_2H_4) constitutes the smallest molecule based on a carbon double bond, which is a fundamental building block for many bigger organic molecules present in nature. Its photochemistry has therefore been subject of intense research. We studied the relaxation dynamics of the ethylene cation with unprecedented temporal resolution by combining few-femtosecond extreme-ultraviolet (XUV) and infrared (IR) pulses. Comparison of the experimental fragment dynamics with ab initio calculations allowed us to identify several ultrafast relaxation channels that unfold on time scales <50 fs. In addition, a precise upper limit for the isomerization time of 30±3 fs was found.

Session: XAS4 – XMCD (15:45-17:15, Auditorium E3)

Nanophases in Complex Oxides
Thu_XAS4_1
Presented by Elke Arenholz
Functional complex oxide materials exhibit characteristics such as magnetism, ferroelectricity, and conduction that can be controlled by applying external fields (electric, magnetic, strain) or other excitations (light, heat, …). Nanoscale heterogeneity – the spontaneous formation of regions with distinct atomic, electronic and/or magnetic order – is a fundamental materials property and its origin and links to functionality are intensely studied and hotly debated. In this talk current opportunities and future directions for characterizing nanophases in functional complex oxides with

soft x rays will be featured and discussed.

Magnetic remanence in Ho adatoms on thin MgO Layers
Thu_XAS4_2
Presented by Sebastian Stepanow
Realizing magnetic remanence in a single atom allows for storing and processing information in the smallest unit of matter. In XMCD experiments we show that individual holmium (Ho) atoms adsorbed on ultrathin MgO(100) layers on Ag(100) exhibit magnetic remanence up to a temperature of 30 kelvin and a relaxation time of 1500 seconds at 10 kelvin. The extraordinary stability is achieved by the realization of a symmetry-protected magnetic ground state, the low phonon density of states of the stiff MgO layer and by decoupling the Ho spin from the underlying metal by a tunnel barrier.

Site-specific valence atomic orbital characterization of magnetic surfaces by angular-momentum-polarized Auger electrons
Thu_XAS4_3
Presented by Fumihiko Matsui
When a core level is excited by circularly polarized light (CPL), angular momentum of light (helicity) is transferred to an emitted photoelectron, which can be confirmed by the parallax shift measurement of forward focusing peak (FFP) direction. Here we report the observation and quantitative analysis of the angular momentum transfer from light to Auger electrons, instead of photoelectron, from Cu surfaces and Ni magnetic thin films. In the case of magnetic materials, circular dichroism in the x-ray absorption intensity (XMCD), was observed together with angular momentum transfer (parallax shift) effect. Magnetic-quantum-number(ml)-resolved XMCD spectra were successfully obtained.

Magnetic circular dichorism of X-ray absorption, emission, and photoemission in spinel-type ferrites
Thu_XAS4_4
Presented by Naomi Kawamura
Magnetic circular dichroism (MCD) of hard X-ray spectroscopy (X-ray absorption, emission, and photoemission) in spinel-type ferrites were performed to investigate the electronic and magnetic states under resonant conditions. High-resolution dichroic signals are provided by combining a high-resolution monochromator with an X-ray phase retarder so that an enhancement of MCD at the pre-edge in X-ray absorption and emission was observed. Otherwise, a resonant effect in the photoemission spectroscopy was little for the MCD signals near the absorption edge. The features of obtained MCD spectra and electronic states in the ferrites are discussed from a viewpoint of X-ray spectroscopy.

Session: In-situ (15:45-17:15, Auditorium E5)

Relaxation Processes in Core-Level Ionized Aqueous Solution: Entanglement of Electronic and Nuclear Dynamics
Thu_InSitu_1
Presented by Bernd Winter
We report on relaxation processes involving simultaneous autoionization and proton transfer between adjacent molecules in aqueous systems, so-called proton transfer mediated charge separation (PTM-CS) process. Within PTM-CS, molecular transients with a half-transferred proton are formed within a few femtoseconds after the core-level ionization event. Subsequent non-radiative decay of the highly non-equilibrium transients leads to a series of reactive species. The non-local electronic decay processes are discussed for several small molecules which form hydrogen bonds with water: water(aq), hydrogen peroxide (aq), ammonia(aq), and ammonium(aq). Identification of the proton dynamics is through isotope effects in the high-energy tail of the Auger-electron spectra.

Short abstracts of talks

***Operando* soft X-ray emission spectroscopy for rechargeable-battery electrodes**
Thu_InSitu_2
Presented by Daisuke Asakura
We have developed *operando* soft X-ray emission spectroscopy (XES) system to understand the electronic-structure change of rechargeable-battery electrodes during the charge/discharge reactions. For $LiMn_2O_4$ cathode, *operando* Mn 2*p* XES spectra reversibly changed due to charge/discharge. The changes are attributed to the redox reaction of $Mn^{3+} \leftrightarrow Mn^{4+}$. The configuration-interaction full-multiplet calculations revealed that the Mn^{4+} state has strong charge-transfer effects between the Mn 3*d* and O 2*p* orbitals.

In operando transmission-type liquid cell for soft X-ray absorption spectroscopy of liquid and electrochemical reaction
Thu_InSitu_3
Presented by Masanari Nagasaka
A transmission-type liquid cell has been developed for soft X-ray absorption spectroscopy (XAS). We have measured transmission-mode XAS of several aqueous solutions by optimizing the liquid thickness in the range of 20 nm to 2000 nm, and revealed their local structures. Furthermore, we have measured in operando XAS of electrochemical reactions by developing a transmission-type liquid cell with built-in electrodes with the same scan rate as in cyclic voltammetry (100 mV/s).

The reactivity of $La_2O_2CO_3$ towards CO_2 investigated with *in situ* HERFD XAS and valence-to-core XES
Thu_InSitu_4
Presented by Ofer Hirsch
$La_2O_2CO_3$ based sensors show a good chemoresistive response to CO_2. The atomic positions within the unit cell and the electronic structure are not known until now. Here we resolve the crystal structure of $La_2O_2CO_3$. We compare the HERFD XAS and vtc XES spectra of $La_2O_2CO_3$ and $La(OH)_3$ and relate differences in the spectra to the resolved crystal structure with FEFF calculations. We in-situ investigate the CO_2 sensing mechanism by HERFD XAS and vtc XES. We analyze the electronic states participating in the charge transfer from $La_2O_2CO_3$ to CO_2. Finally, propose a sensing mechanism by combining resistance measurements and spectroscopic results.

Friday, 8 July 2016

Session: RIXS 4 – AMO (9:00-10:30, Auditorium E3)

X-ray Vibrational and Electronic Spectroscopy of Liquid Water and Solutions with RIXS
Fri_RIXS4_1
Presented by Yoshihisa Harada
High-resolution resonant inelastic X-ray scattering spectra of liquid H_2O, D_2O, obtained by excitation across the O 1s resonance show well-separated multiple vibrational structures in the elastic line region, corresponding to the internal OH stretch vibration in the ground state of water. At pre-edge resonance the energy of the first-order vibrational excitation is strongly blue shifted while at post-edge resonance it is red shifted with respect to the main band in the infrared or Raman spectra of water, indicating that water molecules with a particular hydrogen bond configuration can selectively be excited by tuning the energy of the incident X-ray. It is also demonstrated that this technique can also be applied to probe the vibrational energy of OH species in aqueous solution.

Probing hydrogen bonding orbitals: resonant inelastic soft x-ray scattering of aqueous NH_3
Fri_RIXS4_2
Presented by Lothar Weinhardt
To probe the influence of hydrogen bonding on the electronic structure of ammonia, gas phase and aqueous NH_3 have been investigated using soft x-ray absorption (XAS), resonant inelastic soft x-ray scattering (RIXS), and electronic structure calculations including dynamical effects. Strong spectral differences in the XAS and RIXS spectra between gas phase and aqueous NH_3 are attributed to orbital mixing with the water orbitals, dipole-dipole interactions, and nuclear dynamics on the fs time-scale. All of these effects are consequences of hydrogen bonding, demonstrating the power of XAS and RIXS as unique tools to study hydrogen bonding in liquids.

Ion-solvation-induced molecular reorganization in liquid water probed by resonant inelastic soft X-ray scattering and X-ray emission spectroscopy
Fri_RIXS4_3
Presented by Michael Zharnikov
The molecular structure of liquid water is susceptible to changes upon admixture of salts due to ionic solvation, providing the basis of many chemical and biochemical processes. We demonstrate how the local electronic structure of aqueous salt solutions can be studied by resonant inelastic soft x-ray scattering and x-ray emission spectroscopy to monitor the effects of ion solvation on the hydrogen-bond network of liquid water. Significant changes in the oxygen K-edge emission spectra are observed with increasing salt concentration. They are attributed to modifications in proton dynamics, caused by a specific coordination structure around the salt ions.

Charge transfer parameters of cobalt halides and sulfide derived from cobalt 2p3d RIXS
Fri_RIXS4_4
Presented by Ru-Pan Wang
We provide high resolution 2p3d resonant inelastic X-ray scattering (RIXS) results of CoF_2, $CoCl_2$, $CoBr_2$ and CoS_x. We calculate the 2p3d RIXS spectra of Co^{2+} with different charge transfer energies (Δ) using charge transfer multiplet (CTM) calculations. Comparing the 2p3d RIXS experiment with calculations, we can determine the total crystal field (10Dq) and Δ values. From wavefunction analysis, we provide the ground state nature of the Co^{2+} ions with respect to symmetry and hybridization.

Session: Time res. 2 (9:00-10:30, Auditorium E5)

X-ray coherent diffractive imaging of quantum vortices in superfluid helium droplets
Fri_Time2_1

Presented by Andrey Vilesov
This talk describes recent x-ray coherent diffractive imaging of vortices in superfluid 4-He droplets.

Photoexcited process of WO_3 Photocatalyst in femtoseconds to picoseconds region observed by time-resoled XAFS
Fri_Time2_2
Presented by Yohei Uemura
Photoexcitated states of WO_3 were studied by ultrafast XAFS using PF-AR and SACLA. The photoexcited state of WO_3 was measured at PF-AR. The time resolution of the experiments was about 100 ps. The excited states of WO_3 were successfully observed and the excited state decayed within 10 ns. Faster photoexcitation processes were followed by femtosecond X-rays emitted from SACLA. The edge shift was observed within the 200 ps, followed by the relatively slow changes which corresponded to local structural changes of WO_3.

Transient band gap enhancement in the excitonic insulator phase of Ta_2NiSe_5 upon photoexcitation
Fri_Time2_3
Presented by Claude Monney
By using time- and angle-resolved photoemission spectroscopy (trARPES), we show that the band gap of the semiconductor Ta_2NiSe_5 can be transiently increased on the sub-picosecond timescale with an ultrashort infrared laser pulse. We attribute this remarkable effect to be intimately related to the excitonic insulator phase taking place in this material at low temperature. Our result suggests that for a few hundreds of femtoseconds, an out-of-equilibrium phase takes place upon photoexcitation in which the exciton condensate is enhanced with respect to the thermalized value.

One-step theory of two-photon photoemission with first application to Ag(001)
Fri_Time2_4
Presented by Hubert Ebert
A theoretical frame for two-photon photoemission is presented that is based on the Keldysh formalism. This is used to describe the real-time evolution of the initial states after an arbitrarily strong pump pulse. For two-photon photoemission spectroscopy one may assume that the probe as well as pump pulses are weak. Representing the final states by a time-reversed low-energy electron diffraction state leads to an expression for the photo current very similar to that of Pendry's original formulation of the one-step model. First numerical results of the scheme are presented for Ag(100) with the surface Rydberg states as intermediate states.